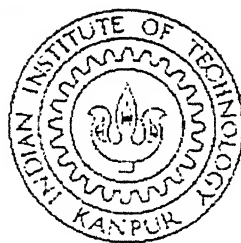


MODELING VAPOR-LIQUID EQUILIBRIA OF REFRIGERANT MIXTURES USING THE WONG-SANDLER MODEL

A thesis submitted
in Partial Fulfillment of the Requirements
for the Degree of
Master of Technology

by

Kalpesh Kumar Pandey



to the


**DEPARTMENT OF CHEMICAL ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY
KANPUR 208016**

MAY, 2000



CERTIFICATE

It is certified that the work contained in the Thesis titled **Modeling Vapor-Liquid Equilibria of Refrigerant Mixtures using the Wong-Sandler Model**, by **Kalpesh Kumar Pandey**, has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.


Dr. R. P. Singh

Professor,

Department of Chemical Engineering

Indian Institute of Technology, Kanpur

May 3, 2000

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ABSTRACT

An ever increasing concern on the stratosphere ozone depletion has led to a world wide ban on chlorofluorocarbons (CFCs) and prompted rigorous search for alternative refrigerants with zero Ozone-Depletion Potential (ODP) and lower Global Warming Potential (GWP). To develop an optimum alternative to replace an existing CFC pure fluid or mixture requires accurate thermodynamic information (especially vapor-liquid equilibrium behavior) of not only the old refrigerants, but also of the possible replacements. In the present study, the capabilities of the Wong-Sandler (WS) model using different G^E equations (NRTL, UNIQUAC, UNIQUAC-R) have been explored in the equation of state (EOS) modeling of isothermal binary vapor-liquid equilibria (VLE) for a vastly extended range of refrigerant mixtures and conditions. The results showed that the WS mixing rule using any of the three G^E equations in all cases could be accurately fitted to binary refrigerant VLE data. Similar results obtained with the UNIQUAC-R and UNIQUAC models strongly suggests that the entropic part (combinatorial term) has little influence on the accuracy of VLE predictions over the range of conditions studied. The WS model showed good convergence ability, which is of vital importance in VLE calculations, due to its robustness to parameter variation. Its accurate extrapolation capabilities would be useful in extending limited experimental data, especially for newer and unconventional refrigerant mixtures.

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NOMENCLATURE

a	cohesion energy parameter in cubic EOS
b	covolume parameter in cubic EOS
a_{ji}	parameters of UNIQUAC model
f^L, f^V	fugacity of component i in liquid and vapor phase
k	parameter as defined in eq.(3.7)
k_0	universal function of acentric factor in eq.(3.8)
k_1	substance specific parameter in eq.(3.7)
k_{ij}, k_{ji}	binary interaction parameter
q_i	surface area parameter of component i
r_i	volume parameter of component i
u_{ij}	average interaction energy
v	molar volume
x	mole fraction of component in a liquid mixture
y	mole fraction of component in a vapor mixture
z	coordination number
A	Helmholtz free energy of mixing
D	defined as in eq.(3.19)
G	Gibbs free energy of mixing
G_{12}, G_{21}	parameters of NRTL activity coefficient model
N	number of data points
P	Pressure
P_c	critical pressure
Q	defined as in eq.(3.18)
Q_k	surface area
R	universal gas constant
R_k	group volume
T	absolute temperature
T_c	critical temperature
Z	compressibility factors

Greek letters

α	nonrandomness parameter of NRTL model
γ_i	activity coefficient of component i
σ	constant of PRSV equation of state
ϕ_i	segment or volume fraction of component i
φ_i	fugacity coefficient of component i
τ_{12}, τ_{21}	parameters of NRTL activity coefficient model
θ_i	area fraction of component i
ω	acentric factor

Superscripts

i,j	pure component property
ij	interaction property between component i and j
E	excess property
L	liquid
V	vapor
∞	infinite pressure property
12	binary property of component 1 and 2

Subscript

i,j	components
EOS	equation of state
c	critical property
r	reduced property

CHAPTER 1

INTRODUCTION

In accord with an increasing concern on the stratospheric ozone depletion, the timetable toward a complete ban on the production and consumption of chlorofluorocarbons (CFCs) and hydrofluorocarbons (HCFCs) has been accelerated to phase them out. The study of the 'ozone hole' above the Antarctic established the relationship between the chlorine and ozone content in the stratospheric zone and dictated that the chlorine oxide (ClO^\cdot) radical is mainly responsible for the ozone destruction. This radical is formed by chlorine atoms released by chlorofluorocarbons (CFCs) and hydrochlorofluorocarbons (HCFCs), used mainly in the refrigeration industry. The environmental regulations that have been imposed on all countries in order to tackle the problem of ozone depletion, forced the refrigeration industry to totally phase out CFCs in 1995, and HCFCs in the following years (2015 for Western Europe) (Clodic and Sauer, 1994). The recommended worldwide ban on many low-molar-mass chlorofluorocarbons has prompted rigorous search for alternatives with zero Ozone-Depletion Potential (ODP) and lower Global Warming Potential (GWP).

The chlorofluorocarbons were primarily used as refrigerants, but are also important as blowing agents in polymer foam manufacture and cleaning solvents in electronic circuit manufacture. In many cases, such as refrigeration applications (which is most important area of use of CFCs), it is necessary to develop alternative fluids with thermodynamic properties which are similar to CFCs they are to replace so that existing equipment can be used with a minimum of modification. For this purpose first hydrofluorocarbons (HFCs) and hydrochlorofluorocarbons (HCFCs) and their mixtures were suggested, though now fluorinated alcohols and their mixtures with HFCs and HCFCs and other fluids are also being considered (Sauermann et al., 1993; Laugier et al., 1994; Nowaczyk and Steimle, 1992). The use of mixtures can result in energetic improvements, extensions of the application range and favourable influence to undesirable properties of one of the components, such as flammability, insolubility in oil or green house effect implications.

For example, whereas HFC-134a is one of the promising candidates as an alternative refrigerant because it contains the hydrogen atom and has short atmospheric life resulting in low ODP and GWP, there are disadvantages in using pure HFC-134a. It has poor compatibility with lubricants due to the absence of chlorine atoms. This disadvantage can be eliminated by mixtures with other refrigerants (e.g. HCFC-124) which have a good compatibility with lubricants. Azeotropic mixtures have merit when used as refrigerants because they show behavior similar to pure components. Thus the list of possible choices for new refrigerant mixtures to replace the CFCs is very large and growing. To develop an optimum alternative to replace an existing CFC pure fluid or mixture requires accurate thermodynamic information (especially vapor-liquid equilibrium behavior) of not only the old refrigerants, but also of the possible replacements. To obtain detailed experimental data for all promising substitutes is expensive and time consuming. Ideally, a predictive model such as UNIFAC would be useful in such cases, at least to screen possible candidate mixtures for their suitability in a specific application. However, recent attempts (Klieber, 1994) indicate that current UNIFAC group definitions and interaction parameters for such fluids are either non-existent or do not lead to accurate predictions.

At present, the best choice for the design engineer is to collect a minimum amount of data at select temperatures and pressures, and then to use these data with a model to extrapolate phase behavior to other temperatures and pressures. The vapor-liquid equilibrium modeling of refrigerant mixtures can be done using either activity coefficient (the so-called gamma-phi) models or equations of state (EOS). Usually EOS modeling is preferable because in refrigeration design not only is VLE important, but so are other thermodynamic properties (such as density and enthalpy) and these can also be obtained from the same EOS model.

In order to accurately correlate and/or predict VLE with equations of state, it is necessary to have an EOS that can represent pure component saturation pressures accurately. There have been significant improvements in the accuracy of cubic EOS for the prediction of pure component properties in the last two decades (Sandler et al., 1994). Much effort in recent years has been devoted toward developing multiparameter mixing rules,

especially those that incorporate the excess free energy (G^E or A^E) to extend the cubic EOS for the phase equilibrium calculations of complex mixtures (Orbey and Sandler, 1995a; Heidemann, 1996). There is a rapidly growing literature exploring techniques for implanting specific G^E behavior into the cubic equation of state through the mixing rules. Models that combine equations of state and G^E models can be categorized into two groups: those that make this link at infinite pressure (Huron and Vidal, 1979; Wong and Sandler, 1992), and those that make this link at low or zero pressure (Mollerup, 1986; Heidemann and Kokal, 1990; Michelsen, 1990_{a,b}, and Dahl and Michelsen, 1990).

Attempts to incorporate excess Gibbs energy model information into equations of state were initiated by Huron and Vidal (1979) who matched the G^E of the solution model to that of the EOS at the state of infinite pressure. However, their mixing rule has not become widely used because the available G^E parameters at low pressures can not be used in their mixing rules. Wong and Sandler (1992) and Wong et al. (1992) incorporated the second virial coefficient as well as solution model into the mixing rule obtained by identifying the excess Helmholtz free energy (A^E) of a solution model into that of an EOS at infinite pressure. Available low-pressure solution model parameters are found to be useful in this mixing rule because of the insensitivity of A^E to pressure. This theoretically correct mixing rule provides a unified and consistent way of combining two-parameter cubic equations of state and excess free energy models to describe the phase behavior of a wide variety of mixtures. The Wong-Sandler model has a broad range of applicability; it can be used as a multiparameter correlative model to accurately fit phase equilibrium data of highly non ideal mixtures (Wong and Sandler, 1992), or it can be used as a predictive model (Wong et al., 1992, Orbey et al., 1993) with parameters obtained from G^E information available in data banks.

In this work, the capabilities of the Wong-Sandler (WS) model have been explored in the EOS modeling of isothermal binary vapor-liquid equilibria for a vastly extended range of refrigerant mixtures and conditions. Following Deiters (1997), Table 1 presents the engineering nomenclature ('R nomenclature') as defined by ASHRAE (American Society of Heating, Refrigeration, and Air Conditioning Engineers), the chemical formula, and

Table 1: Refrigerant nomenclature

S.N.	R Nomenclature	Chemical formula	IUPAC name
1	R-12	CFCl_2H	Dichlorofluoromethane
2	R-13	CClF_3	Chlorotrifluoromethane
3	R-22	CF_2ClH	Chlorodifluoromethane
4	R-23	CF_3H	Trifluoromethane
5	R-32	CF_2H_2	Difluoromethane
6	R-40	CClH_3	Chloromethane
7	R-13B1	CF_3Br	Monobromotrifluoromethane
8	R-114	$\text{CF}_2\text{ClCF}_2\text{Cl}$	1,2-Dichloro-1,1,2,2-Tetrafluoroethane
9	R-116	CF_3CF_3	Perfluoroethane
10	R-123	$\text{CFCl}_2\text{CF}_2\text{H}$	Dichlorotrifluoroethane
11	R-124	CFClHCF_3	1-Chloro-1,2,2,2-Tetrafluoroethane
12	R-125	CHF_2CF_3	pentafluoroethane
13	R-134a	CF_3CFH_2	1,1,1,2-Tetrafluoroethane
14	R-140a	CCl_3CH_3	1,1,1-Trichloroethane
15	R-141b	CFCl_2CH_3	1,1-Dichloro-1-Fluoroethane
16	R-142b	CF_2ClCH_3	1-Chloro-1,1-Difluoroethane
17	R-143a	CF_3CH_3	1,1,1-Trifluoroethane
18	R-150a	CCl_2HCH_3	1,1-Dichloroethane
19	R-152a	CF_2HCH_3	1,1-Difluoroethane
20	R-236fa	CF_3CF_3	1,1,1,3,3,3-Hexafluoropropane
21	R-290	$\text{CH}_3\text{CH}_2\text{CH}_3$	Propane
22	R-600a	C_4H_{10}	Isobutane

the IUPAC name of all the refrigerants involved in the 37 systems of binary refrigerant mixtures of CFCs, HCFCs, HFCs, and HCs studied. Liquid phase G^E (activity coefficient) models incorporated in the EOS/ G^E approach are the commonly used NRTL, UNIQUAC and UNIQUAC-R models, where the UNIQUAC-R refers to the activity coefficient model that incorporates only the residual part of the UNIQUAC model. It is recognized that, attractive forces are related only to the residual part of the UNIQUAC model (Brandani et al., 1998). The results indicate that the combinatorial part of the UNIQUAC model has little influence on the accuracy of phase equilibrium calculations in the pressure range of interest.

CHAPTER 2

LITERATURE REVIEW

Owing to their ozone-depleting properties, chlorofluorocarbons (CFCs) are now regulated under the Montreal Protocol (Kruse and Hesse, 1988). Several hydrofluorocarbons (HFCs) are now considered as alternative refrigerants that are harmless or less harmful to the ozone layer. These refrigerants usually form a nonazeotropic mixture, which has recently been considered as the prospective working fluid for refrigeration and heat pump systems resulting in improved coefficient of performance (Kruse, 1981). In order to select the optimal mixture composition for design and operation, it is necessary to know the basic thermodynamic data, especially vapor-liquid equilibria. However, only a few systems have been investigated up to now. At present, the best choice for the design engineer is to collect a minimum amount of VLE data at selected temperatures and pressures and then use these data with a model to extrapolate phase behavior to other temperatures and pressures.

The vapor-liquid equilibrium modeling of refrigerant mixtures can be done using either activity coefficient (the so-called gamma-phi) models or equations of state (EOS). Usually EOS modeling is preferable because in refrigeration design not only is VLE important, but so are other thermodynamic properties (such as density and enthalpy) and these can be obtained from the same EOS model. In order to accurately correlate and/or predict VLE with equations of state, it is necessary to have an EOS that can represent pure component saturation pressures correctly. In recent years several such equations have been suggested (Sandler et al., 1994). Cubic equations of state (EOS) are widely used for thermodynamic property modeling in industrial design, and have proven to be extremely effective (Mathias and Klotz, 1994). They allow a consistent description of phase behavior for mixtures. The extension of a cubic, two-parameter EOS to mixtures requires mixing rules for the parameters. For relatively simple mixtures, it is common to use the van der Waals (vdW) one-fluid mixing rules. VLE data for the CFCs are relatively easy to correlate with cubic equations of state using the conventional one-

parameter van der Waals (vdW) mixing rules. Also, at least in the narrow ranges of temperature, their phase behavior is predictable with only one temperature-independent binary interaction parameter (Abu-Eishah, 1991; Moshfegian et al, 1992; Gow, 1993; Kleiber, 1994; Lee et al., 1996; Chung and Kim, 1997; Lee et al., 1998). Moreover, it is feasible to correlate the binary parameter with temperature for each binary system (Gow, 1993). Nonetheless, a global correlation applicable for all binaries is difficult to achieve, as noted by Abu-Eishah (1991). An alternative approach is to correlate the binary parameter with pure component parameters, such as the acentric factor or compressibility factor, as shown by Lee and Sun (1992). However, with a growing number of new refrigerant mixtures, including alcohol-containing mixtures (Laugier et al., 1994), and the increased ranges of temperature and pressure of interest, this approach is no longer adequate for vapor-liquid equilibrium (VLE) information.

In recent years, much effort has been given to the incorporation of the excess Gibbs free energy G^E models into mixing rule expressions for the attractive term parameter of cubic equation of state, as it allows description of vapor-liquid equilibria (VLE) in complex systems through a simple EOS (Orbey and Sandler, 1995a; Heidemann, 1996). There is a rapidly growing literature exploring techniques for implanting specific G^E behavior into the cubic equation of state through the mixing rules (EOS- G^E framework). The need for alternative refrigerant systems brought up the requirement for predictive models over a range of conditions, which need only a few experimental data in order to estimate their parameters. . Appropriate candidate models that can meet this need are based on the G^E -EOS formalism (Orbey and Sandler, 1995a). Advantages of this approach are the built-in temperature dependence of the parameters of the G^E model, and the ability to utilize diverse experimental information, as for example excess enthalpy (H^E) experimental data (Peng et al., 1995).

Models that combine equations of state and activity coefficient (or G^E) models can be categorized into two groups: those that make this link at infinite pressure (Huron and Vidal, 1979; Wong and Sandler, 1992), and those that make this link at low or zero pressure (Mollerup, 1986; Heidemann and Kokal, 1990; Michelsen, 1990_{a,b}; and Dahl

and Michelsen, 1990). Of these, the Wong-Sandler (WS) mixing rules have shown remarkable extrapolating powers and gained wide acceptance. Wong and Sandler (1992) and Wong et al. (1992) incorporated the second virial coefficient as well as solution model into the mixing rule obtained by incorporating the excess Helmholtz free energy (A^E) of a solution model into that of an EOS at infinite pressure. Available low-pressure solution model parameters are found to be useful in this mixing rule because of the insensitivity of A^E to pressure. This theoretically correct mixing rule provides a unified and consistent way of combining two-parameter cubic equations of state and excess free energy models to describe the phase behavior of a wide variety of mixtures and has a broad range of applicability. Summarizing in the words of Sandler and Orbey (1998), "Wong and Sandler have developed a mixing rule that combines an EOS with a free energy model but produces the desired EOS behavior at both low and high densities without being density dependent, uses the existing tables of G^E parameters, allows extrapolation over wide ranges of temperature and pressure, and provides a conceptually simple method of accurately extending UNIFAC or other low-pressure VLE prediction methods to high temperature and pressure". The original paper has been followed with a number of publications by Sandler and his coworkers, including Wong et al. (1992), Pividal et al. (1992), Orbey et al. (1993), Huang et al. (1994), Orbey and Sandler (1995a, d), Orbey and Sandler (1996), Orbey and Sandler (1997) and Shiflett and Sandler (1998).

Orbey and Sandler (1995d) have tested the temperature extrapolation capabilities of the conventional vdW and three recently introduced multiparameter mixing rules for a cubic equation of state to predict the VLE behavior of some CFC, HCFC, and fluorinated alcohol binary mixtures. The multiparameter mixing rules considered were the three-parameter mixing rule of Wong and Sandler (1992), a two-parameter empirical mixing rule introduced by Stryjek and Vera (1986b) and various other investigators (Adachi and Sugie, 1986; Panagiotopoulos and Reid, 1986) and then developed into a multiparameter form by Schwartzentruber and Renon (1989), and a new form of a two-parameter modified Huron-Vidal mixing rule (Sandler and Orbey, 1995a). Of particular interest was determining how well these mixing models could correlate experimental data at a single temperature, and then how accurately each could predict phase behavior at other

temperatures with temperature independent parameters. The results indicate that for some new refrigerant mixtures only the excess free energy based equation of state mixing rules (Wong and Sandler, 1992, Orbey and Sandler, 1995a) can provide acceptable correlations, and also reasonable predictions over a wide range of temperatures. While all the models considered performed well for conventional refrigerant mixtures, only the excess free-energy based models consistently led to accurate predictions over wide-ranges of temperature; the other models result in less accurate predictions and, in some cases, false liquid-liquid splitting.

Recently, Ioannidis and Knox (1997) have presented a single energy parameter model for several traditionally used and recently proposed refrigerant mixtures based on the Wong-Sandler mixing rule. The solution model used is a modification of G^E model based on the work of Knox et al. (1984), that assigns one energy and one size related parameter per binary mixture. The system studied include fluorocarbons (FCs), CFC, and HCFC mixtures and CFC/HCFC-hydrocarbon mixtures.

Shiflett and Sandler (1998) have modeled seven binary fluorocarbon mixtures forming azeotropes using the Wong-Sandler mixing rules with the nonrandom-two liquid (NRTL) activity coefficient model (Renon and Prausnitz, 1968). The azeotropes consisted of binary mixtures of HFCs, FCs, carbon dioxide, ammonia, and propane. These azeotropes demonstrate a variety of nonideal behavior including polar/polar, polar/nonpolar, and nonpolar/nonpolar interactions, and in some cases large molecular size differences. These systems provided a challenging test for the Wong-Sandler mixing rule.

CHAPTER 3

THERMODYNAMIC MODELING

3.1 Criterion for vapor-Liquid Equilibrium

The criterion that must be satisfied for components at equilibrium between liquid and vapor phases at the same temperature (T) and pressure (P) is given by the equality of component fugacities throughout the phases.

$$f_i^V = f_i^L \quad (3.1)$$

The liquid-vapor-phase component fugacities can both be described through fugacity coefficients:

$$f_i^L = x_i \phi_i^L P = f_i^V = y_i \phi_i^V P \quad (3.2)$$

The liquid-phase fugacity coefficient of a component i in a mixture, ϕ_i^L , is given by

$$\ln \phi_i^L = \frac{1}{RT} \int_{V^L}^{\infty} \left[\left(\frac{\partial P}{\partial n_i} \right)_{T,V,n_j} - \frac{RT}{V^L} \right] dV - \ln Z^L \quad (3.3)$$

where Z^L is the liquid compressibility factor.

Similarly the vapor-phase fugacity coefficient of a component i in a mixture, ϕ_i^V , is given by

$$\ln \phi_i^V = \frac{1}{RT} \int_{V^V}^{\infty} \left[\left(\frac{\partial P}{\partial n_i} \right)_{T,V,n_j} - \frac{RT}{V^V} \right] dV - \ln Z^V \quad (3.4)$$

where Z^V is the vapor compressibility factor.

A suitable pressure-explicit EOS, $P=f(V,T)$ applicable to all pure components and their mixtures over the entire density range (vapor to liquid) is required for the solution of Eqs. (3.3) and (3.4).

3.2 Cubic Equation of State

The PRSV equation of state used in this study is the Peng-Robinson EOS modified by Stryjek and Vera(1986a):

$$P = \frac{RT}{v-b} - \frac{a(T)}{v(v+b)+b(v-b)} \quad (3.5)$$

where v is the molar volume, R the universal gas constant, a and b the characteristic mixture energy and size (covolume) parameters, respectively. Pure component parameters a and b are obtained from Eqs. (3.6) through (3.9) from critical temperature T_c , critical pressure P_c , acentric factor ω , and an adjustable parameter k ; characteristic of each pure component:

$$a(T) = 0.457235 \frac{R^2 T_c^2}{P_c} \left[1 + k(1 - T_r^{0.5}) \right]^2 \quad (3.6)$$

where $T_r = T/T_c$

$$k = k_0 + k_1(1 + T_r^{0.5})(0.7 - T_r) \quad (3.7)$$

$$k_0 = 0.378893 + 1.4897153\omega - 0.17131848\omega^2 + 0.0196554\omega^3 \quad (3.8)$$

$$b = 0.077796 \frac{RT_c}{P_c} \quad (3.9)$$

The PRSV equation of state is applicable to a wide variety of non-polar, polar and associating substances.

For the PRSV equation of state and arbitrary set of mixing rules for mixture parameters a and b , the fugacity coefficient of component i in a mixture is given by

$$\ln \phi_i = -\ln \left[\frac{P(v-b)}{RT} \right] + \frac{1}{b} \left(\frac{\partial nb}{\partial n_i} \right) \left(\frac{Pv}{RT} - 1 \right) + \frac{1}{2\sqrt{2}} \left(\frac{a}{bRT} \right) \left[\frac{1}{a} \left(\frac{1}{n} \frac{\partial}{\partial} \frac{n^2 a}{n_i} \right) - \frac{1}{b} \left(\frac{\partial}{\partial} \frac{nb}{n_i} \right) \right] \cdot \ln \left[\frac{v+b(1-\sqrt{2})}{v+b(1+\sqrt{2})} \right] \quad (3.10)$$

3.3 Mixing Rules: The Wong-Sandler (WS) Model

The development of Wong-Sandler mixing rules is based on two observations. The first is the quadratic composition dependence of the second virial coefficient. This provides one of the restrictions on the equation of state a and b parameters, given by

$$b - \frac{a}{RT} = \sum_i \sum_j x_i x_j \left(b - \frac{a}{RT} \right)_{ij} \quad (3.11)$$

For the combining rule, various possibilities exist. In the original work, Wong and Sandler used

$$\left(b - \frac{a}{RT} \right)_{ij} = \frac{1}{2} \left[\left(b - \frac{a}{RT} \right)_i + \left(b - \frac{a}{RT} \right)_j \right] (1 - k_{ij}) \quad (3.12)$$

which introduces a second virial coefficient binary interaction parameter k_{ij} ($k_{ij}=k_{ji}$).

The second observation is that the excess Helmholtz free energy of mixing (A^E) is much less pressure dependent than the excess Gibbs free energy (G^E).

$$G^E(T, x_i, P = low) = A^E(T, x_i, P = low) = A^E(T, x_i, P = high) \quad (3.13)$$

The first of these equalities follows from the fact that $G^E = A^E + PV^E$, and the PV^E term is very small at low pressures. The second of these equalities is a result of the essential pressure (or density) independence of A^E . The second equation for the a and b parameters

then comes from the condition that

$$A_{EOS}^E(T, x_i, P = \infty) = A^E(T, x_i, P = \infty) = A^E(T, x_i, P = low) = G^E(T, x_i, P = low) \quad (3.14)$$

Here the subscript EOS refers to the excess Helmholtz free energy derived from an equation of state, while G^E and A^E without subscript refer to a free energy or activity coefficient model. Combining these, the basic relation for the Wong-Sandler rule for the mixture parameters a and b of a cubic equation of state are

$$b - \frac{a}{RT} = \sum_i \sum_j x_i x_j \left(b - \frac{a}{RT} \right)_{ij} \quad (3.11)$$

and

$$\frac{A_{\infty}^E}{\sigma} = \frac{a}{b} - \sum_i x_i \frac{a_i}{b_i} \quad (3.15)$$

where A^E is an excess Helmholtz free energy term, and as a result of Eq. (3.14) above, any G^E (activity coefficient) model can be used for A^E . Here σ is a constant dependent on the specific EOS selected; $(1/2^{0.5})\ln(2^{0.5}-1)=-.62323$ for the PRSV equation used here. The parameters in this mixing rule are those of the A^E model and the binary interaction parameter k_{ij} appearing in the combining rule, Eq. (3.12).

Equations (3.11) and (3.15), together with Eq. (3.12), completely define a and b in terms of A_{∞}^E (the high-density term) and k_{ij} (the low-density term). These equations can be solved to obtain

$$b = \frac{\sum_i \sum_j x_i x_j \left(b - \frac{a}{RT} \right)_{ij}}{1 - \frac{A_{\infty}^E}{RT\sigma} - \sum_i x_i \left(\frac{a_i}{b_i RT} \right)} = \frac{Q}{1-D} \quad (3.16)$$

and

$$\frac{a}{RT} = \frac{b}{RT} \left[\sum_i x_i \frac{a_i}{b_i} + \frac{A_{\infty}^E}{\sigma} \right] = Q \left(\frac{D}{1-D} \right) \quad (3.17)$$

with Q and D defined as

$$Q = \sum_i \sum_j x_i x_j \left(b - \frac{a}{RT} \right)_{ij} \quad (3.18)$$

and

$$D = \sum_i x_i \frac{a_i}{b_i RT} + \frac{A_\infty^E}{RT\sigma} \quad (3.19)$$

Using the Wong-Sandler mixing rules given by Eqs. (3.16) and (3.17), the partial derivatives of a and b required in Eq. (3.10) for calculating $\ln \phi_i$ are:

$$\frac{\partial nb}{\partial n_i} = \frac{1}{(1-D)} \left(\frac{1}{n} \frac{\partial n^2 Q}{\partial n_i} \right) - \frac{Q}{(1-D)^2} \left(1 - \frac{\partial nD}{\partial n_i} \right) \quad (3.20)$$

and

$$\frac{1}{RT} \left(\frac{1}{n} \frac{\partial n^2}{\partial n_i} \right) = D \frac{\partial nb}{\partial n_i} + b \frac{\partial nD}{\partial n_i} \quad (3.21)$$

with the partial derivatives of Q and D given by :

$$\frac{1}{n} \frac{\partial n^2 Q}{\partial n_i} = 2 \sum_j x_j \left(b - \frac{a}{RT} \right)_{ij} \quad (3.22)$$

$$\frac{\partial nD}{\partial n_i} = \frac{a_i}{b_i RT} + \frac{\ln \gamma_{\infty i}}{\sigma} \quad (3.23)$$

with

$$\ln \gamma_{\infty i} = \frac{1}{RT} \frac{\partial n A_\infty^E}{\partial n_i} \quad (3.24)$$

3.4 Activity Coefficient Models: Binary Systems

3.4.1 NRTL (non-random two liquid) Model:

In Non-Random-Two-Liquid (NRTL) model of Renon and Prausnitz (1968), the molar excess Gibbs free energy for a binary mixture is given as

$$\frac{G^E}{RT} = x_1 x_2 \left[\frac{\tau_{21} G_{21}}{x_1 + G_{21} x_2} + \frac{\tau_{12} G_{12}}{G_{12} x_1 + x_2} \right] \quad (3.25)$$

where

$$\tau_{12} = \frac{g_{12} - g_{22}}{RT}, \quad \tau_{21} = \frac{g_{21} - g_{11}}{RT}$$

$$G_{12} = \exp(-\alpha \tau_{12}), \quad G_{21} = \exp(-\alpha \tau_{21}),$$

The activity coefficients are given by

$$\ln \gamma_1 = x_2^2 \left[\tau_{21} \left(\frac{G_{21}}{x_1 + G_{21} x_2} \right)^2 + \frac{\tau_{12} G_{12}}{(x_2 + G_{12} x_1)^2} \right] \quad (3.26)$$

$$\ln \gamma_2 = x_1^2 \left[\tau_{12} \left(\frac{G_{12}}{x_2 + G_{12} x_1} \right)^2 + \frac{\tau_{21} G_{21}}{(x_1 + G_{21} x_2)^2} \right] \quad (3.27)$$

It is a three parameter (α , τ_{12} , and τ_{21}) model in which α is a non-randomness parameter.

3.4.2 UNIQUAC (UNiversal QUAsi Chemical) Model:

The UNIQUAC model of Abrams and Prausnitz (1975) is

$$\frac{G^E}{RT} = \frac{G^E}{RT}(\text{combinatorial}) + \frac{G^E}{RT}(\text{residual}) \quad (3.28)$$

where

$$\frac{G^E}{RT}(\text{combinatorial}) = x_1 \ln \frac{\phi_1}{x_1} + x_2 \ln \frac{\phi_2}{x_2} + \frac{z}{2} \left(q_1 x_1 \ln \frac{\theta_1}{\phi_1} + q_2 x_2 \ln \frac{\theta_2}{\phi_2} \right) \quad (3.29)$$

$$\frac{G^E}{RT}(\text{residual}) = -q_1 x_1 \ln(\theta_1 + \theta_2 \tau_{21}) - q_2 x_2 \ln(\theta_2 + \theta_1 \tau_{12}) \quad (3.30)$$

$$\phi_i = \text{segment or volume fraction of component } i = \left(\frac{x_i r_i}{\sum_j x_j r_j} \right)$$

$$\theta_i = \text{area fraction of component } i = \left(\frac{x_i q_i}{\sum_j x_j q_j} \right)$$

r_i = volume parameter of component i ;

q_i = surface area parameter of component i ;

$$\tau_{ji} = \exp \left\{ -\frac{u_{ji} - u_{ii}}{RT} \right\} = \exp \left(-\frac{a_{ji}}{T} \right) = \text{adjustable parameter};$$

u_{ij} = average interaction energy for the interaction of molecules of component i with the molecules of component j ; and

z = coordination number which is usually taken as 10.

The activity coefficients are given by

$$\ln \gamma_i = \ln \gamma_i^C(\text{combinatorial}) + \ln \gamma_i^R(\text{residual}) \quad (3.31)$$

$$\ln \gamma_i^C = \ln \frac{\phi_i}{x_i} + \frac{z}{2} q_i \ln \frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i} \sum_j x_j l_j \quad (3.32)$$

$$\ln \gamma_i^R = q_i \left[1 - \ln \left(\sum_j \theta_j \tau_{ji} \right) - \sum_j \frac{\theta_j \tau_{ij}}{\left(\sum_k \theta_k \tau_{kj} \right)} \right] \quad (3.33)$$

where $l_i = \frac{z}{2}(r_i - q_i) - (r_i - 1)$

The structural parameters r_i and q_i can be calculated as the sum of the group volume and area parameters R_k and Q_k .

$$r_i = \sum_k v_k^{(i)} R_k \quad (3.34)$$

$$q_i = \sum_k v_k^{(i)} Q_k \quad (3.35)$$

where $v_k^{(i)}$ is the number of groups of type k in a molecule of component i .

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Pure Component Constants and Mixture VLE Data

Table 4.1 gives the literature source of isothermal VLE data for 37 binary refrigerant mixtures. The critical temperature (T_c), critical pressure (P_c), and acentric factor (ω), for each component in the mixture, taken from the references given in Table 4.1, are provided in Table 4.2. A computer program was used to evaluate the k_1 constant of the PRSV equation of state by minimizing the overall deviation in vapor pressure (AAD). The k_1 constant and the AAD are both provided in Table 4.2 together with the literature source of vapor pressure data. The overall deviation in pressure is calculated using the following formula

$$AAD = \frac{1}{N} \sum \left(\frac{|P_{exp} - P_{cal}|}{P_{exp}} \right) 100 \quad (4.1)$$

where N is the number of data points, P_{exp} is measured pressure, and P_{cal} is the calculated pressure.

4.2 Data Reduction

In the Wong-Sandler mixing rule the EOS parameters for a homogeneous liquid or vapor mixture is computed from Eqs. (3.16), (3.17) together with Eq. (3.12). The single adjustable parameter k_{ij} [Eq. (3.12)] for each binary pair is referred to as the WS mixing rule parameter (k_{12}). Three excess free energy (or equivalently activity coefficient) models were evaluated for calculating G^E : NRTL, UNIQUAC, UNIQUAC-R. Parameters τ_{12}, τ_{21} for each binary mixture are referred to as the G^E model parameters. The values of the pure component parameters r_i, q_i in the UNIQUAC model were taken from Ioannidis and Knox (1997) or calculated from the group contribution parameters R_k, Q_k , respectively, given by Fredenslund and Sorensen (1994). The NRTL model has the additional advantage of having a third adjustable parameter, α . This is typically set to a

Table 4.1 Literature source of experimental VLE data for refrigerant mixtures (contd.).

No	System	N	T (K)	P Range (MPa)	Reference
1.	R-32+R-143a	13	256.00	0.35-0.45	Shiflett and Sandl (1998)
2.	R-32+R-116	14	253.55	1.056-0.4108	Shiflett and Sandl (1998)
3.	R-32+R-125	11 14	257.85 284.40	0.4008-0.4815 0.9459-1.1477	Shiflett and Sandl (1998)
4.	R-32+R-290	11	257.85	0.2863-0.4815	Shiflett and Sandl (1998)
5.	R-23+R-116	12 15	209.60 227.60	0.2094-0.2681 0.4398-0.5737	Shiflett and Sandl (1998)
6.	R-32+R-134a	5 5 5 5 5 5 5	263.15 273.15 283.15 293.15 303.15 313.15 323.15	0.1997-0.579 0.2916-0.810 0.414-1.104 0.5709-1.471 0.769-1.9227 1.015-2.474 1.316-3.136	Chung and Kim (1997)
7.	R-125+R-134a	6 8 4 8 7	268.15 273.15 278.15 283.15 293.15	0.254-0.544 0.308-0.633 0.415-0.689 0.442-0.882 0.606-1.0158	Kobayashi and Nishiumi (1998)
8	R32+R-125	6 5 5 4	283.05 293.05 303.05 313.05	0.915-1.104 1.202-1.48 1.563-1.923 2.001-2.477	Chung and Kim (1997)
9.	R-22+R-12	11 18	356.15 343.81	2.413-3.88 1.869-3.01	Nishumi et al.(1995)
10.	R-22+R-123	13 13 14 12	414.57 383.15 353.92 333.70	1.785-5.813 0.985-5.158 0.49-3.216 0.279-2.381	Nishumi et al.(1995)
11.	R-134a+R-124	6 9 8	296.45 302.25 307.25	3.7-6.21 4.31-7.48 4.98-8.65	Lee et al. (1996)
12.	R-124+R-142b	12 11	298.15 312.15	3.38-3.79 5.08-5.73	Lee et al. (1996)

Table 4.1 Literature source of experimental VLE Data for refrigerant mixtures (contd.).

No	System	N data	T (K)	P Range (MPa)	Reference
13.	R-142b+R-141b	13	323.4	0.185-0.6846	Kang and Lee (1990)
14.	R-142b+R-140a	13	323.4	0.0465-0.6846	Kang and Lee (1990)
15.	R-141b+R-140a	14	323.4	0.0465-0.185	Kang and Lee (1990)
16.	R-32+R-22	13	283	0.6722-1.1035	Kang and Chung. (1996)
17.	R-32+R-12	16	283	.4204-1.1035	Kang and Chung (1996)
18.	R-32+R-40	13	283	.3619-1.1035	Kang and Chung (1996)
19.	R-134a+R-141b	5 6 7 11	278.15 288.15 318.15 333.15	0.101-0.269 0.101-0.389 0.221-0.999 0.34-1.504	Zheng et al.(1990)
20.	R-23+R-13	16 18 18 21	272.944 249.66 224.611 199.6388	1.96-2.49 1.218-1.499 .446-.513 .154-.164	Stein and Proust. (1971)
21.	R-134a+R-123	6 7 8 10	289.17 303.15 318.15 332.74	0.12-0.393 0.201-0.628 0.278-1.096 0.476-1.495	Kubota et al.(1991)
22.	R-22+R-114	5 8 12 19	253.15 283.15 313.15 338.15	0.076-0.229 0.181-0.619 0.616-1.175 0.799-2.594	Kubota et al.(1990a)
23.	R-12+R-114	10 10	283.15 313.15	0.18-0.394 0.387-0.896	Kubota et al.(1990a)
24.	R-13B1+R-12	5 18 12	253.15 283.15 313.15	0.207-0.411 0.463-1.066 1.069-2.087	Kubota et al.(1990a)
25.	R-22+R-142b	15 16 16 21 18 13	263.15 273.15 283.15 293.15 313.15 338.15	0.098-0.355 0.146-0.498 0.21-0.679 0.293-0.824 0.526-1.534 0.995-2.704	Kubota et al.(1990b)
26.	R-32+R-142b	8 8 8	295.45 304.55 314.95	0.31-1.571 0.409-1.998 0.549-2.558	Lee et al.(1998)

Table 4.1 Literature source of experimental VLE data for refrigerant Mixtures.

No	System	N data	T (K)	P Range (MPa)	Reference
27.	R-32+R123	9	294.95	.0816-1.554	Lee et al.(1998)
		9	304.55	.116-1.998	
		10	313.95	.159-2.527	
28	R-134a+R600a	17	293.66	0.3067-0.58	Bobbo et al. (1998)
		11	303.68	0.41-0.7809	
29.	R-134a+R-236fa	9	283.62	0.162-0.42	Bobbo et al. (1998)
		10	303.68	0.325-0.78	
30.	R600a+R236fa	15	303.68	0.325-0.41	Bobbo et al. (1998)
31.	R-22+R23	8	273.15	0.7152-3.55	Roth et al. (1992)
		7	293.15	1.11-3.85	
		8	303.15	1.525-4.8	
		8	323.15	2.4-5.2	
32.	R-152a+R-150a	10	303.2	.134-.685	Lim et al. (1996)
		10	323.2	.158-1.147	
33.	R-134a+R-142b	10	268.0	.1189-.2425	Klieber. (1994)
		11	283.0	.2066-.4132	
		11	298.0	.3365-.6622	
34.	R-134a+R-12	10	258	.1815-.1631	Klieber (1994)
		10	278	.3602-.3485	
		10	298	.6477-.6622	
35.	R-134a+R-152a	8	255	.1306-.1438	Klieber (1994)
		8	275	.2821-.3129	
		9	298	.5936-.6622	
36.	R-134a+R-116	10	251	.9804-.1210	Klieber (1994)
		8	275	1.1709-.3129	
37.	R-14+R-13	12	199.80	.1544-1.5272	Proust and Stein. (1979)
38.	R-22+R-134a	7	273.16	.2925-.4983	Arita et al. (1991)
		6	298.16	.6651-1.0445	
		7	323.16	1.3173-1.9420	

Table 4.2: Critical temperatures and pressures, acentric factor, k_1 and overall pressure deviation (contd.).

S.N.	Component	$T_c(K)$	$P_c(MPa)$	ω	k_1	AAD(%)	T range (K)	References
1	R-116	293.140	3.060	0.2554	-0.0101	0.2660	209.6-253.55	Shifflet and Sandler (1998)
2	R-23	299.070	4.836	0.2652	0.0030	0.3120	199.6-272.94	Shifflet and Sandler (1998), Stein and Proust (1971)
3	R-32	351.600	5.814	0.2759	-0.0651	0.0120	208.36-348.63	Weber and Goodwin (1993), Holcomb et al. (1993)
4	R-125	339.170	3.617	0.3048	-0.0121	1.0090	220.00-337.99	Duarte-Garza et al. (1997b)
5	R-134a	374.300	4.070	0.3270	-0.0231	0.5580	199.99-390.18	Maezawa et al (1990), Niesen et al. (1994), Maezawa et al. (1991)
6	R-22	369.300	4.970	0.2210	0.0150	1.3000	313.06-333.16	Kohlen et al.(1985)
7	R-123	456.510	3.672	0.2350	-0.2828	0.3299	279.97-453.14	Maezawa et al (1990),Weber (1990), Piao et al. (1991)
8	R-124	395.700	3.630	0.2860	0.0097	0.3990	310.94-394.50	Niesen et al. (1994)
9	R-142b	410.260	4.040	0.2300	0.0440	0.2364	210.0-300.05	Silva and Weber (1993), Maezawa et al. (1991a)
10	R-141b	477.310	4.250	0.2210	0.1160	0.4980	253.82-370.0	Defibaugh et al.(1993), Duarte-garza et al. (1997a), Maezawa et al. (1991)
11	R-140a	545.000	4.240	0.2140	0.1160	0.5120	297.00-443.1	Yada et al. (1991)
12	R-12	384.920	4.129	0.1790	-0.1524	0.5010	213.19-383.92	Michels et al. (1966), Fernandez-Fassnacht and del Rio (1985)
13	R-40	416.270	6.700	0.1530	0.0066	0.1130	283.000	Kang and chung (1996)

Table 4.2: Critical temperatures and pressures, acentric factor, k_1 and overall pressure deviation

S.N.	Component	T_c (K)	P_c (MPa)	ω	k_1	AAD(%)	T range (K)	References
14	R-143a	346.310	3.760	0.2523	0.0108	0.2460	263.5-353.16	Nakamura et al. (1997)
15	R-114	418.780	3.248	0.2510	-0.1044	0.0260	253.15-338.15	Kubota et al. (1990a)
16	R-13B1	340.080	3.963	0.1730	-0.1211	1.0160	253.15-313.15	Kubota et al. (1990a)
17	R-600a	408.130	3.648	0.1830	0.0026	0.0540	293.66-303.68	Bobbo et al. (1998)
18	R-236fa	403.750	3.180	0.2913	0.0054	1.2060	283.62-303.68	Bobbo et al. (1998)
19	R-152a	386.600	4.500	0.2560	0.1452	0.4085	219.92-378.10	Silva and Weber (1993), Holcomb et al. (1993)
20	R-150a	523.000	5.100	0.2400	0.0258	0.6200	303.2-323.2	Lim et al (1996)
21	R-13	302.000	3.870	0.1980	0.1078	0.7573	188.22-380.2	Michels et al. (1966), Fernandez-Fassnacht and del Rio (1985)
22	R-290	369.850	4.2447	0.1523	0.0029	0.1810	257.85	Shifflet and Sandler (1998)

fixed value of 0.3 for vapor-liquid equilibria. In the case of few binary mixtures such as R-32/R-134a, R-32/R-125 and R-32/R-290, an α value of 0.2 was found to provide a better fit which is consistent with the highly nonideal liquid-liquid equilibria at high temperatures. A three parameter fit of the isothermal VLE data using the WS mixing rules with the G^E models (k_{12} , τ_{12} , τ_{21}) was performed. The computer program used a simplex algorithm to optimize G^E model parameters (τ_{12} and τ_{21}) and the WS mixing rule parameter (k_{12}). The VLE calculations presented here were done using an isothermal bubble point algorithm. A flow diagram of the algorithm is presented in Fig. 4.1. When optimizing the model parameters, the following objective function was used

$$F = \sum_i |P_{i,exp} - P_{ical}| \quad (4.2)$$

for the minimization in a simplex formalism.

The WS model showed good convergence ability, which is of vital importance in VLE calculations, due to its robustness to parameter variation. The program used for correlating the data required an initial guess for each parameter. The initial values of τ_{12} , τ_{21} and k_{12} were chosen to be 0.1. The program was run and fitted parameters along with the calculated pressure and vapor composition were computed. To ensure that a global vs. a local minimum convergence was obtained, values of τ_{12} , τ_{21} and k_{12} were varied in increments of 0.01. The calculated τ_{12} , τ_{21} and k_{12} which provided the best fit with the experimental data were identified as the optimum set of parameters and are presented in Table 4.3. The optimum set of UNIQUAC parameters were used also in VLE calculations with the UNIQUAC-R model to assess the sensitivity of the entropic term (combinatorial part) on phase equilibrium predictions.

4.3 Results and Discussion

Tables 4.4 through 4.8 give the VLE results for five systems for which only P-x data were available; measured and calculated pressures and the calculated vapor compositions are presented along with percent average absolute deviation in pressure. Figures 4.2

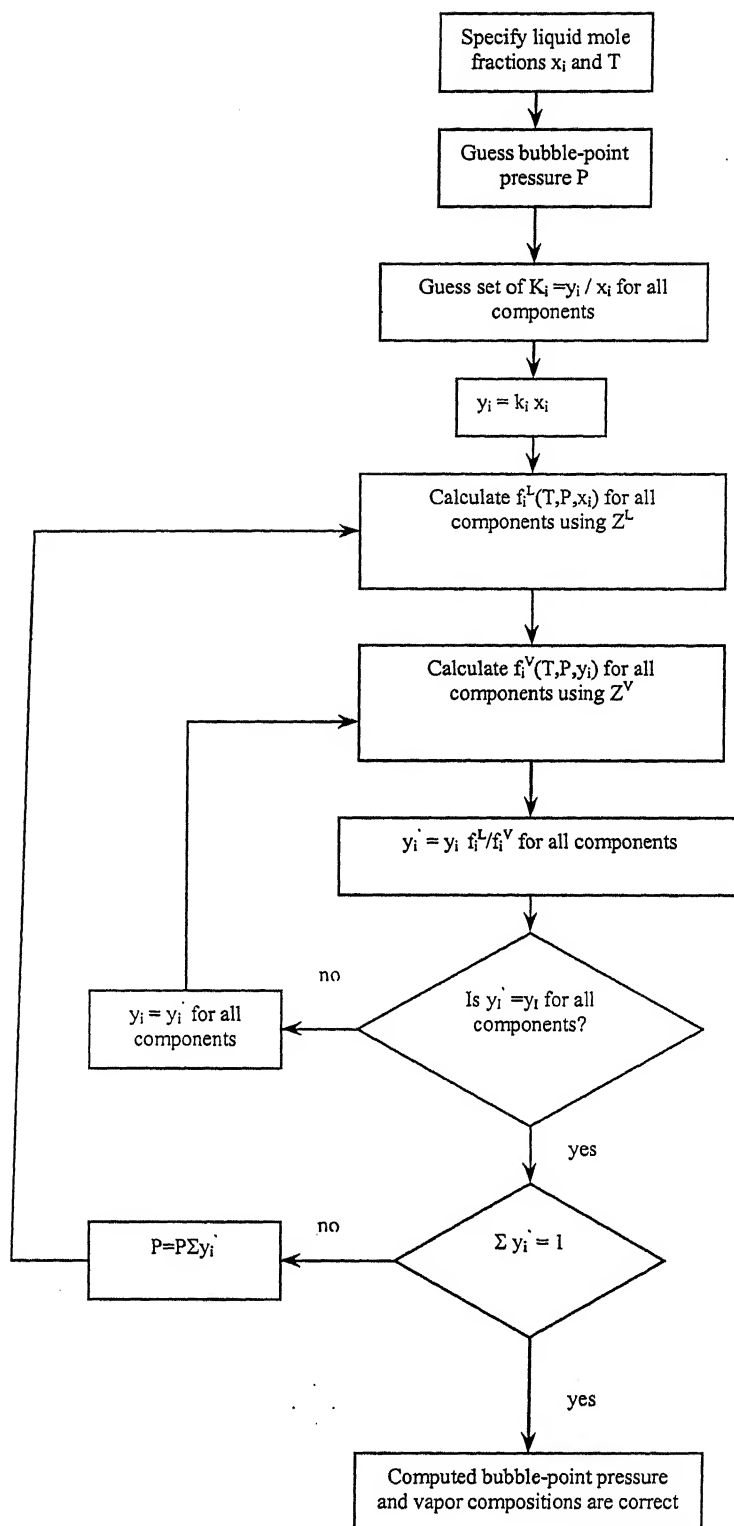


Fig. 4.1 Isothermal bubble pressure algorithm

Table 4.3: Calculated EOS, NRTL and UNIQUAC parameters (contd.).

S.N.	MIXTURE	T (K)	NRTL model				UNIQUAC model			
			k_{12}	α	τ_{12}	τ_{21}	k_{12}	τ_{12}	τ_{21}	
1	HFC-32/HFC-143a	256.00	0.1004	0.3	0.3200	0.0695	0.3411	2.1034	0.4100	
2	HFC-32/FC-116	253.55	0.5211	0.3	1.4311	0.1512	0.2893	0.5676	0.0337	
3	HFC-32/HFC-125	284.40	0.1219	0.3	-0.0107	0.0423	0.3116	2.7338	0.2473	
		257.85	0.1003	0.3	-0.0251	0.1000	0.2091	2.7290	0.1000	
4	HFC-32/HC290	257.85	0.0227	0.2	3.7193	1.8865	0.2000	0.0930	0.1000	
5	HFC-23/FC-116	209.60	0.1183	0.3	1.0312	1.2704	0.2011	0.8200	0.0948	
		227.60	-0.1608	0.3	1.7947	1.5327	0.1005	0.7200	0.1032	
6	HFC-32/HFC-134a	263.15	0.1999	0.2	-0.5100	0.0809	0.2012	2.8213	0.0900	
		273.15	0.0999	0.2	-0.1835	0.0938	0.2016	2.0056	0.3640	
		283.15	0.1010	0.2	-0.1964	0.1000	0.2997	2.6849	0.2544	
		293.15	0.0998	0.2	-0.2412	0.0690	0.2638	2.7749	0.1951	
		303.15	0.1007	0.2	-0.2564	0.0786	0.2027	2.8218	0.0950	
		313.15	0.0991	0.2	-0.2359	0.1098	0.1994	2.8200	0.0994	
		323.15	0.1000	0.2	-0.2636	0.1144	0.2006	2.9200	0.0945	
7	HFC-125/HFC-134a	268.15	0.1010	0.3	-0.3433	0.1127	0.1002	2.2914	0.3018	
		273.15	0.1000	0.3	-0.3100	0.0880	0.1287	2.2497	0.3291	
		278.15	0.1000	0.3	-0.3300	0.1008	0.1010	2.8214	0.1157	
		283.15	0.1000	0.3	-0.3348	0.0979	0.1154	2.2546	0.3215	
		293.15	0.1001	0.3	-0.3229	0.0986	0.1000	2.2200	0.3200	
8	HFC-32/HFC-125	283.05	0.1000	0.2	0.0941	0.0991	0.1010	2.1200	0.1331	
		293.05	0.1000	0.2	0.0396	0.1017	0.1005	2.2200	0.1217	
		303.05	0.0997	0.2	-0.0100	0.0855	0.1010	2.2200	0.1460	
		313.05	0.1004	0.2	-0.0617	0.1076	0.1183	2.4098	0.1215	
9	HFC-22/ICFC-12	356.15	0.1335	0.3	-0.4056	0.6581	0.3111	2.9570	0.1450	
		343.81	-0.1155	0.3	0.2730	0.7370	0.1003	1.9473	0.3010	

Table 4.3: Calculated EOS, NRTL and UNIQUAC parameters (contd.).

S.N.	MIXTURE	T (K)	NRTL model				UNIQUAC model			
			k_{12}	α	τ_{12}	τ_{21}	k_{12}	τ_{12}	τ_{21}	
10	HCFC-22/HCFC-123	414.57	0.1961	0.3	-0.4005	0.1194	0.1643	1.9900	0.3166	
		383.15	0.2103	0.3	-0.3064	0.0801	0.2358	2.5940	0.1718	
		353.92	0.2005	0.3	-0.4497	0.0900	0.2668	2.8963	0.1602	
		333.70	0.1824	0.3	-0.4349	0.1282	0.2318	2.6923	0.1968	
11	HFC-134a/HCFC-124	296.45	0.1006	0.3	-0.2100	0.1362	0.1021	2.1200	0.3162	
		302.25	0.0999	0.3	-0.0880	0.0988	0.1481	2.1228	0.3357	
		307.25	0.1000	0.3	-0.0784	0.1085	0.1747	2.2577	0.3011	
12	HCFC-124/HCFC142b	298.15	0.0983	0.3	-0.4336	0.0572	0.1000	2.3207	0.3136	
		312.15	0.2856	0.3	-0.4493	-0.5165	0.1002	2.4200	0.2789	
13	HCFC-142b/HCFC141b	323.40	0.1006	0.3	-0.1455	0.0944	0.1033	1.6909	0.5082	
14	HCFC-142b/HCC-140a	323.40	0.1447	0.3	0.2371	0.0347	0.1832	1.6201	0.4865	
15	HCFC-141b/HCC-140a	323.40	0.1004	0.3	-0.0482	0.1000	0.1897	1.7822	0.4977	
16	HFC-32/HCFC-22	283.00	0.1000	0.3	-0.2100	0.1028	0.2782	2.8651	0.2339	
17	HFC-32/CFC-12	283.00	-0.0296	0.3	1.8712	1.0465	0.2385	0.9879	0.1151	
18	HFC-32/HCC-40	283.00	0.1000	0.3	0.5919	0.0890	0.2097	1.5139	0.3620	
19	HFC-134a/HCFC-141b	278.15	0.4991	0.3	-0.8100	0.0801	0.4485	2.6565	0.2024	
		288.15	0.4880	0.3	-0.5238	-0.2792	0.3348	2.0849	0.2914	
		318.15	0.1307	0.3	0.5934	-0.0696	0.2160	1.6695	0.4089	
		333.15	0.1680	0.3	0.4828	-0.1438	0.1514	1.1465	0.6669	
20	HFC-23/CFC-13	273.94	0.1000	0.3	1.5649	0.1041	0.5153	2.6884	0.1761	
		249.66	0.0024	0.3	3.0525	1.6174	0.0120	0.2406	0.3970	
		224.61	0.0680	0.3	1.1789	0.9274	0.4479	1.6670	0.3576	
		199.64	0.1774	0.3	0.3309	0.8932	0.3469	1.8250	0.2299	

Table 4.3: Calculated EOS, NRTL and UNIQUAC parameters (contd.).

S.N.	MIXTURE	T (K)	NRTL model				UNIQUAC model		
			k_{12}	α	τ_{12}	τ_{21}	k_{12}	τ_{12}	τ_{21}
21	HFC-134a/HCF123	289.17	0.1004	0.3	0.0412	0.0937	0.3176	2.0281	0.4881
		303.15	0.2184	0.3	0.1853	-0.3565	0.2841	2.3950	0.2694
		318.15	0.2056	0.3	-0.6718	0.5891	0.2486	1.7752	0.4946
		332.74	0.2220	0.3	0.2638	-0.3838	0.2680	2.1106	0.3496
22	HCFC-22/CFC-114	253.15	0.4013	0.3	-0.1845	0.0955	0.4990	2.9200	0.1006
		283.15	0.2597	0.3	0.4688	-0.1021	0.4568	2.8508	0.0941
		313.15	0.2764	0.3	1.2003	-0.7900	0.4323	3.0152	0.0526
		338.15	0.1624	0.3	0.8483	-0.0224	0.3908	2.7997	0.0810
23	CFC-12/CFC-114	283.15	0.1005	0.3	-0.0482	0.0000	0.1005	2.0207	0.3012
		313.15	0.0996	0.3	0.0547	0.0738	0.1336	2.0345	0.3014
24	FC-13B1/CFC-12	253.15	0.0145	0.3	-0.2653	0.0946	0.0799	2.5437	0.2273
		283.15	0.1770	0.3	-0.4334	0.0814	0.2285	2.9988	0.1280
		313.15	0.0989	0.3	-0.2100	0.1051	0.1486	2.5052	0.2120
25	HCFC-22/HCF142b	263.15	0.1000	0.3	-0.3530	0.0920	0.1758	2.7949	0.1909
		273.15	0.0996	0.3	-0.3573	0.0887	0.1472	2.7981	0.1373
		283.15	0.0195	0.3	0.0349	0.0502	0.1398	2.6805	0.1509
		293.15	0.0281	0.3	-0.0170	0.0915	0.1671	2.8554	0.1301
		313.15	-0.0741	0.3	0.2527	0.1147	0.1335	2.8374	0.1384
		338.15	0.1000	0.3	-0.3526	0.0807	0.1649	2.9286	0.1357
26	HFC-32/HCF142b	295.45	0.1880	0.3	0.7618	-0.4125	0.3082	1.6918	0.3897
		304.55	0.2351	0.3	0.0716	-0.0032	0.2880	1.6445	0.4916
		314.95	0.1000	0.3	0.4933	0.0815	0.0354	0.6180	0.5952
27	HFC-32/HFC-123	294.95	0.2131	0.3	1.3431	-0.4619	0.2433	1.0859	0.3524
		304.55	0.2509	0.3	1.0464	-0.4334	0.3144	1.3085	0.3087
		313.95	0.2629	0.3	0.3536	0.0161	0.3429	1.6748	0.2476

Table 4.3: Calculated EOS, NRTL and UNIQUAC parameters (contd.).

S.N.	MIXTURE	T (K)	NRTL model				UNIQUAC model			
			k_{12}	α	τ_{12}	τ_{21}	k_{12}	τ_{12}	τ_{21}	
28	HFC-134a/HC-600a	293.66 303.68	0.1640 -0.1515	0.3 0.3	1.1251 2.1624	1.1449 1.5872	0.5576 0.4199	2.0009 1.4047	0.2307 0.4067	
29	HFC-134a/HC-236fa	283.62 303.68	0.0990 0.0996	0.3 0.3	-0.3848 -0.3100	0.1037 0.0939	0.1473 0.1031	2.9782 2.7897	0.1119 0.0000	
30	HC-600a/HC-236fa	303.68	0.1721	0.3	1.2777	0.7289	0.5570	1.5238	0.4816	
31	HCFC-22/HCFC-23	273.15 293.15 303.15 323.15	0.1005 0.0669 0.0933 0.0060	0.3 0.3 0.3 0.3	0.3188 0.2316 -0.1651 -0.0599	0.1389 -0.0293 0.1011 0.1473	0.1000 0.1332 0.1042 0.0108	1.8545 2.4935 2.6200 1.8279	0.1000 0.1582 0.1088 0.3811	
32	HFC-152a/HCC-150a	303.20 323.20	0.1012 0.1000	0.3 0.3	0.2727 0.0658	0.1100 0.0993	-0.0128 0.2997	2.0686 0.8971	0.4894 2.7269	
33	HFC-134a/HCFC-142b	268.00 283.00 298.00	0.0994 0.1005 0.1011	0.3 0.3 0.3	-0.0230 -0.0609 -0.0809	0.1000 0.1024 0.0930	0.2001 0.2199 0.2102	2.2301 2.3434 2.3208	0.3021 0.2884 0.2993	
34	HFC-134a/CFC-12	258.00 278.00 298.00	-0.1520 0.0980 -0.2540	0.3 0.3 0.3	1.0882 1.2760 1.1725	1.1875 0.1111 1.5842	0.4649 0.4301 0.3998	2.0056 2.0461 2.0629	0.3559 0.3159 0.3000	
35	HFC-134a/HFC-152a	255.00 275.00 298.00	0.1000 0.0999 0.1000	0.3 0.3 0.3	-0.5100 -0.5316 -0.5639	0.0919 0.0951 0.1092	0.3989 0.2987 0.1248	3.5534 3.1571 1.9440	0.3076 0.3075 0.5685	
36	HFC-134a/FC-116	251.00 275.00	0.1589 0.4983	0.3 0.3	0.3295 -0.1957	1.5304 0.1000	0.2009 0.2010	1.2329 1.2926	0.3020 0.3000	
37	FC-14/CFC-13	199.80	0.0882	0.3	0.2924	0.1579	0.2133	2.4917	0.1621	
38	HCFC-22/HFC-134a	273.16 298.16 323.16	0.0994 0.1000 0.0997	0.3 0.3 0.3	-0.1728 -0.1725 -0.2216	0.1047 0.1057 0.0889	0.2268 0.1032 0.1420	3.0200 2.6571 2.4457	0.1180 0.1000 0.2387	

Table 4.4: Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-143a(2) mixtures at 256.0 K with different g^E models.

x ₁	y ₁			exptl	P(MPa)		
	calc				calc		
	NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
0.000	0.000	0.000	0.000	0.351	0.351	0.351	
0.074	0.113	0.113	0.113	0.368	0.365	0.368	
0.152	0.219	0.220	0.220	0.386	0.388	0.385	
0.222	0.303	0.306	0.306	0.400	0.402	0.400	
0.288	0.375	0.379	0.379	0.411	0.410	0.412	
0.350	0.436	0.440	0.441	0.422	0.423	0.422	
0.465	0.538	0.541	0.541	0.437	0.437	0.438	
0.569	0.622	0.621	0.621	0.448	0.449	0.448	
0.664	0.694	0.692	0.692	0.454	0.453	0.454	
0.750	0.762	0.759	0.758	0.458	0.457	0.457	
0.829	0.827	0.825	0.825	0.459	0.455	0.457	
0.902	0.894	0.894	0.894	0.458	0.456	0.455	
1.000	1.000	1.000	1.000	0.450	0.449	0.450	
				%AAD	0.333	0.170	
						0.195	

%AAD = average absolute deviation -- defined as $(\sum abs((exp - calc) / exp) * 100) / N$

R-32(1)/R-143a(2) at 256.0 K

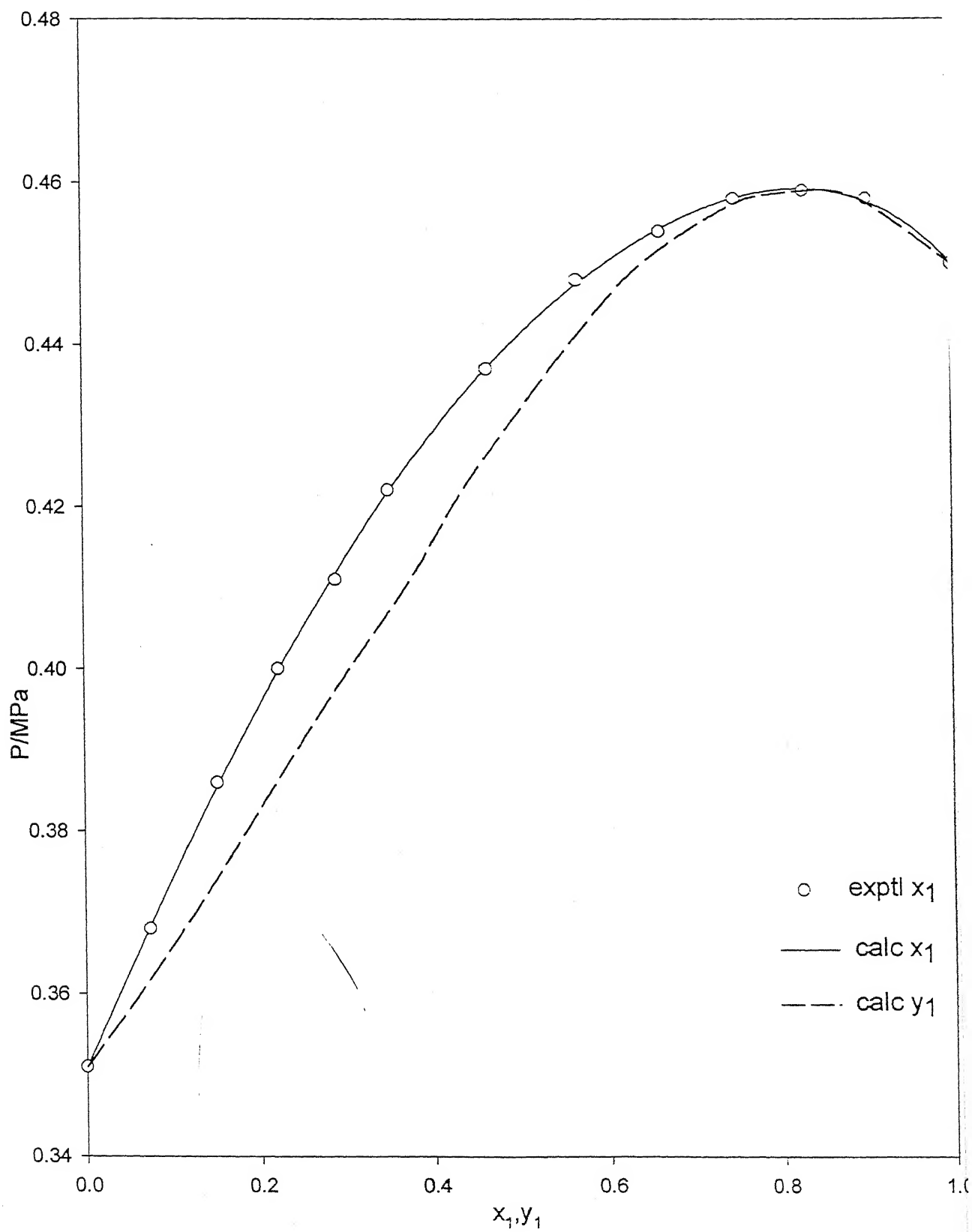


Fig.4.2 Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-143a(2) mixtures at 256.0 K.

Table 4.5: Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-116(2) mixtures at 253.55 K with different g^E models.

x_1	y_1			exptl	P(MPa)		
	calc				calc		
	NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
0.000	0.000	0.000	0.000	1.059	1.058	1.058	1.058
0.056	0.087	0.110	0.110	1.159	1.110	1.170	1.169
0.127	0.175	0.180	0.180	1.221	1.158	1.224	1.224
0.198	0.240	0.227	0.227	1.246	1.186	1.246	1.246
0.268	0.284	0.260	0.261	1.252	1.196	1.250	1.250
0.326	0.306	0.281	0.283	1.248	1.196	1.245	1.245
0.394	0.320	0.299	0.301	1.239	1.192	1.236	1.234
0.485	0.322	0.315	0.318	1.223	1.191	1.221	1.216
0.615	0.311	0.328	0.332	1.198	1.209	1.200	1.193
0.761	0.312	0.348	0.351	1.152	1.202	1.155	1.145
0.855	0.358	0.389	0.391	1.053	1.083	1.052	1.045
0.914	0.443	0.459	0.460	0.903	0.903	0.903	0.899
0.960	0.603	0.597	0.598	0.695	0.679	0.697	0.695
1.000	0.998	0.998	0.998	0.411	0.412	0.412	0.412
				%AAD	2.831	0.236	0.372

%AAD = average absolute deviation defined as $(\sum \text{abs}(\text{exp} - \text{calc}) / \text{exp}) * 100) / N$

R-32(1)/R-116(2) at 253.55 K

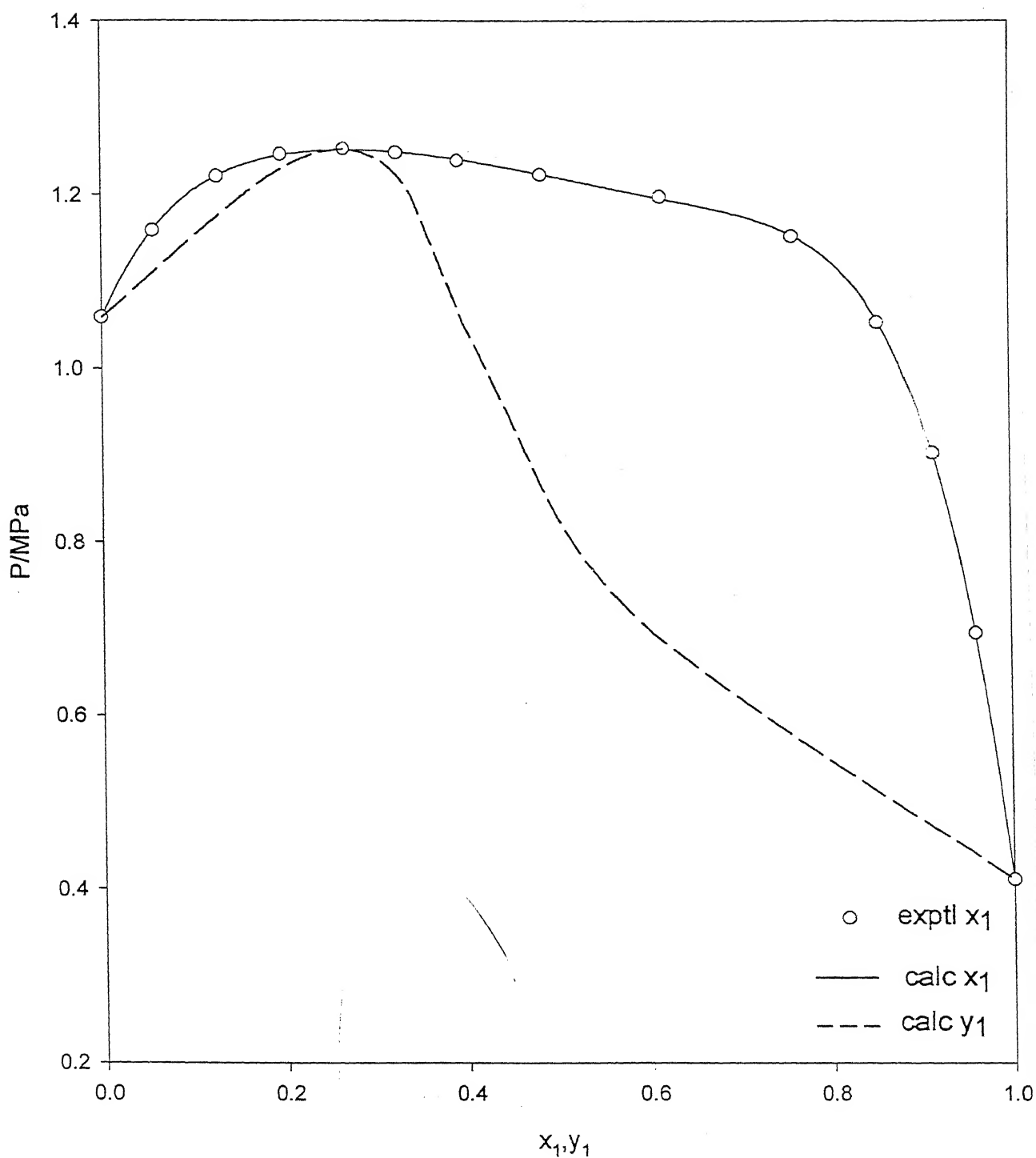


Fig. 4.3 Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-116(2) mixtures at 253.55 K.

Table 4.6: Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-125(2) mixtures with different g^E models.

x_1	y_1			exptl	P(MPa)		
	calc				calc		
	NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
284.4							
0.000	0.000	0.000	0.000	0.946	0.942	0.942	0.942
0.108	0.136	0.136	0.137	0.985	0.984	0.982	0.982
0.204	0.247	0.250	0.250	1.018	1.017	1.016	1.016
0.289	0.339	0.343	0.344	1.044	1.044	1.044	1.044
0.366	0.416	0.422	0.423	1.066	1.067	1.067	1.067
0.435	0.483	0.488	0.489	1.083	1.084	1.085	1.086
0.497	0.540	0.545	0.545	1.098	1.099	1.100	1.100
0.554	0.592	0.595	0.595	1.110	1.111	1.111	1.112
0.654	0.681	0.681	0.681	1.128	1.128	1.128	1.128
0.738	0.754	0.753	0.753	1.139	1.139	1.137	1.138
0.811	0.819	0.818	0.818	1.146	1.145	1.143	1.143
0.874	0.877	0.877	0.877	1.149	1.148	1.146	1.146
0.929	0.929	0.930	0.930	1.150	1.150	1.147	1.147
1.000	1.000	1.000	1.000	1.148	1.148	1.148	1.148
				%AAD	0.088	0.181	0.190

%AAD = average absolute deviation – defined as $(\sum abs((exp - calc) / exp) * 100) / N$

R-32(1)/ R-125(2) at 284.4 K

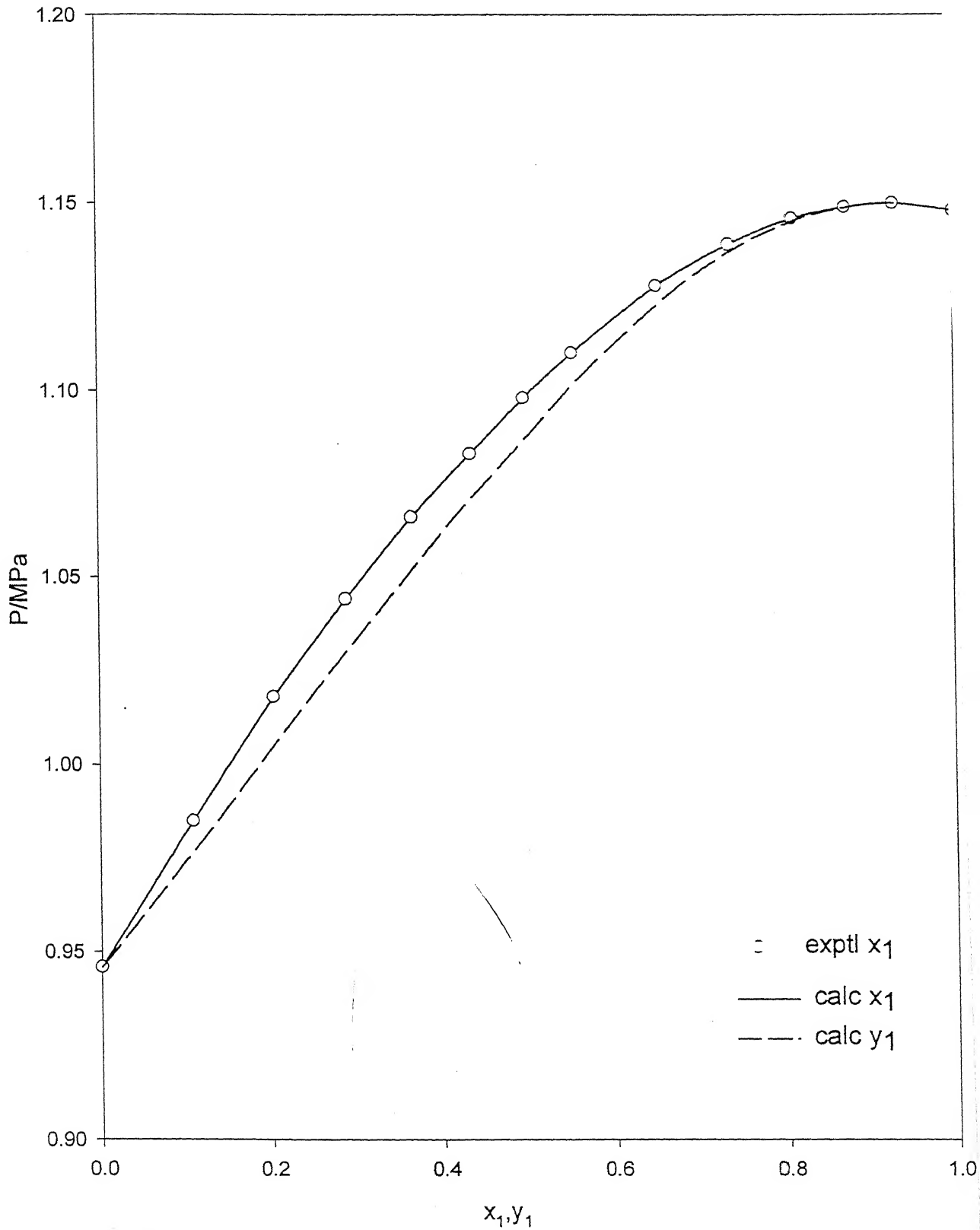


Fig. 4.4 Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-125(2) mixtures at 284.4 K

Table 4.6: Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-125(2) mixtures with different g^E models (contd.).

x_1	y_1				P(MPa)			
	calc				exptl		calc	
	NRTL	UNIQUAC	UNIQUAC-R				NRTL	UNIQUAC
				257.85				UNIQUAC-R
0.000	0.000	0.000	0.000		0.401		0.400	0.400
0.193	0.238	0.239	0.239		0.424		0.428	0.440
0.346	0.399	0.385	0.385		0.444		0.447	0.455
0.495	0.541	0.522	0.523		0.460		0.461	0.464
0.587	0.623	0.607	0.608		0.468		0.468	0.469
0.654	0.682	0.670	0.670		0.474		0.473	0.471
0.704	0.726	0.717	0.717		0.476		0.476	0.473
0.791	0.803	0.800	0.800		0.481		0.479	0.475
0.861	0.866	0.868	0.868		0.483		0.481	0.477
0.931	0.932	0.935	0.935		0.483		0.482	0.479
1.000	1.000	1.000	1.000		0.482		0.482	0.482
					%AAD		0.300	1.106

%AAD = average absolute deviation – defined as $(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100) / N$

R-32(1)/R-125(2) at 257.85 K

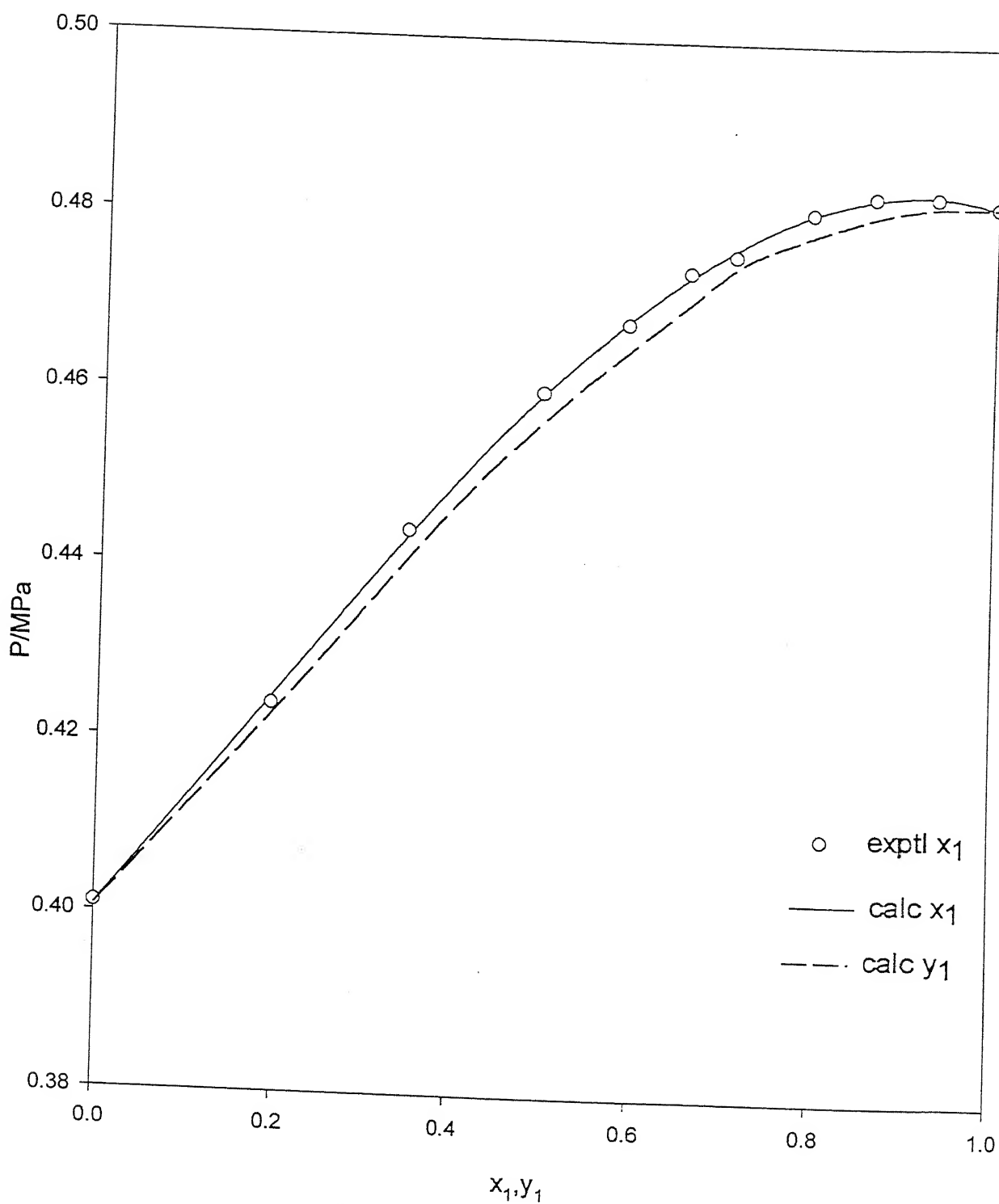


Fig. 4.7 Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-125(2) mixtures at 257.85 K

Table 4.7: Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-290(2) mixtures at 257.85 K with different g^E models.

x_1	y_1			P(MPa)				
	calc			exptl	calc			
	NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R	
0.000	0.000	0.000	0.000	0.286	0.288	0.288	0.288	
0.086	0.431	0.405	0.404	0.491	0.502	0.471	0.471	
0.175	0.536	0.527	0.525	0.601	0.601	0.571	0.569	
0.267	0.583	0.590	0.587	0.658	0.651	0.631	0.629	
0.361	0.611	0.629	0.627	0.686	0.677	0.668	0.666	
0.459	0.632	0.657	0.656	0.698	0.693	0.691	0.690	
0.560	0.649	0.679	0.678	0.702	0.702	0.704	0.704	
0.651	0.661	0.693	0.694	0.708	0.704	0.708	0.709	
0.772	0.670	0.705	0.706	0.702	0.703	0.708	0.708	
0.884	0.684	0.700	0.703	0.667	0.694	0.711	0.709	
1.000	0.999	0.995	0.995	0.482	0.482	0.485	0.485	
				%AAD	0.986	2.351	2.443	

$AAD = \text{average absolute deviation} = \left(\sum \frac{abs((exp - calc) / exp) * 100}{N} \right) / N$

R-32(1)/R-290(2) at 257.85 K

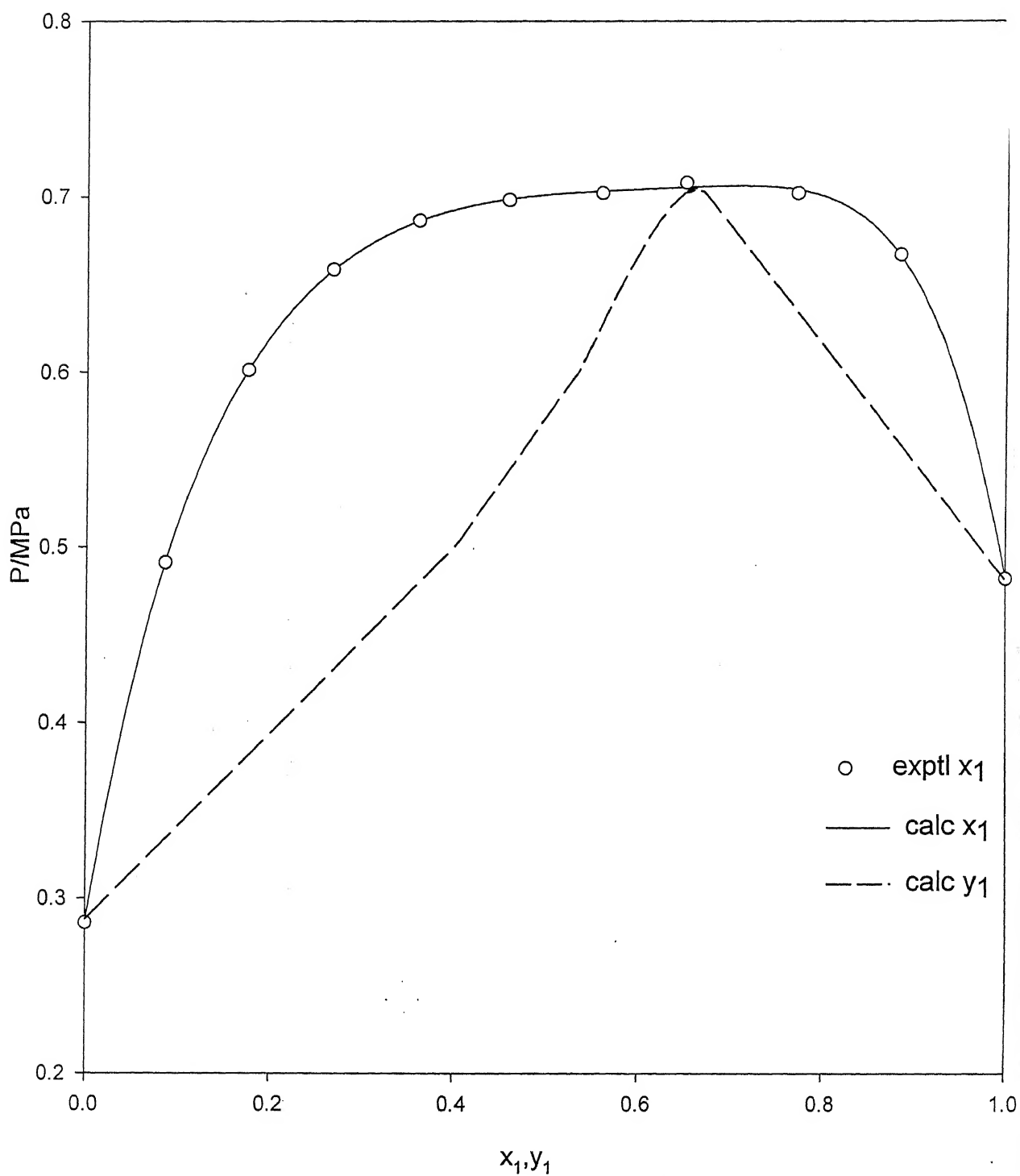


Fig. 4.6 Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-290(2) mixtures at 257.85 K.

Table 4.8: Vapor-liquid equilibrium pressures and phase compositions for R-23(1)/R-116(2) mixtures at 209.6 K with different g^E models (contd.).

x ₁	y ₁			P(MPa)			
	calc			exptl	calc		
	NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
209.6							
0.000	0.000	0.000	0.000	0.209	0.208	0.208	0.209
0.126	0.331	0.332	0.332	0.287	0.287	0.290	0.289
0.196	0.406	0.401	0.400	0.310	0.309	0.310	0.310
0.332	0.491	0.485	0.484	0.333	0.333	0.332	0.332
0.458	0.541	0.539	0.539	0.342	0.342	0.342	0.342
0.537	0.568	0.569	0.569	0.345	0.345	0.344	0.344
0.650	0.610	0.612	0.613	0.344	0.344	0.344	0.344
0.701	0.632	0.634	0.635	0.342	0.342	0.342	0.342
0.761	0.663	0.665	0.666	0.338	0.338	0.338	0.338
0.868	0.748	0.747	0.748	0.321	0.321	0.322	0.322
0.947	0.863	0.860	0.861	0.295	0.295	0.296	0.296
1.000	1.000	1.000	1.000	0.268	0.265	0.266	0.265
				%AAD	0.171	0.335	0.234

%AAD = average absolute deviation – defined as $(\sum abs((exp - calc) / exp) * 100) / N$

Table 4.8: Vapor-liquid equilibrium pressures and phase compositions for R-23(1)/R-116(2) mixtures with different g^E models.

x ₁	y ₁			P(MPa)			
	calc			exptl	calc		
	NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
227.6							
0.000	0.000	0.000	0.000	0.440	0.438	0.438	0.438
0.040	0.132	0.137	0.136	0.496	0.495	0.498	0.498
0.079	0.216	0.219	0.219	0.535	0.538	0.540	0.540
0.133	0.295	0.297	0.297	0.583	0.582	0.583	0.583
0.148	0.312	0.315	0.314	0.590	0.593	0.593	0.592
0.213	0.374	0.377	0.376	0.627	0.628	0.627	0.627
0.261	0.410	0.414	0.413	0.647	0.648	0.646	0.646
0.287	0.428	0.432	0.432	0.660	0.657	0.655	0.655
0.495	0.547	0.553	0.554	0.704	0.701	0.698	0.698
0.533	0.568	0.573	0.574	0.707	0.704	0.702	0.702
0.691	0.655	0.657	0.658	0.701	0.703	0.702	0.702
0.784	0.716	0.715	0.717	0.688	0.690	0.690	0.690
0.843	0.763	0.762	0.763	0.675	0.674	0.675	0.675
0.918	0.846	0.843	0.843	0.639	0.641	0.643	0.643
1.000	1.000	1.000	1.000	0.574	0.575	0.575	0.575
				%AAD	0.593	0.713	0.694

%AAD = average absolute deviation – defined as $\left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$

R-23(1)/R-116(2)

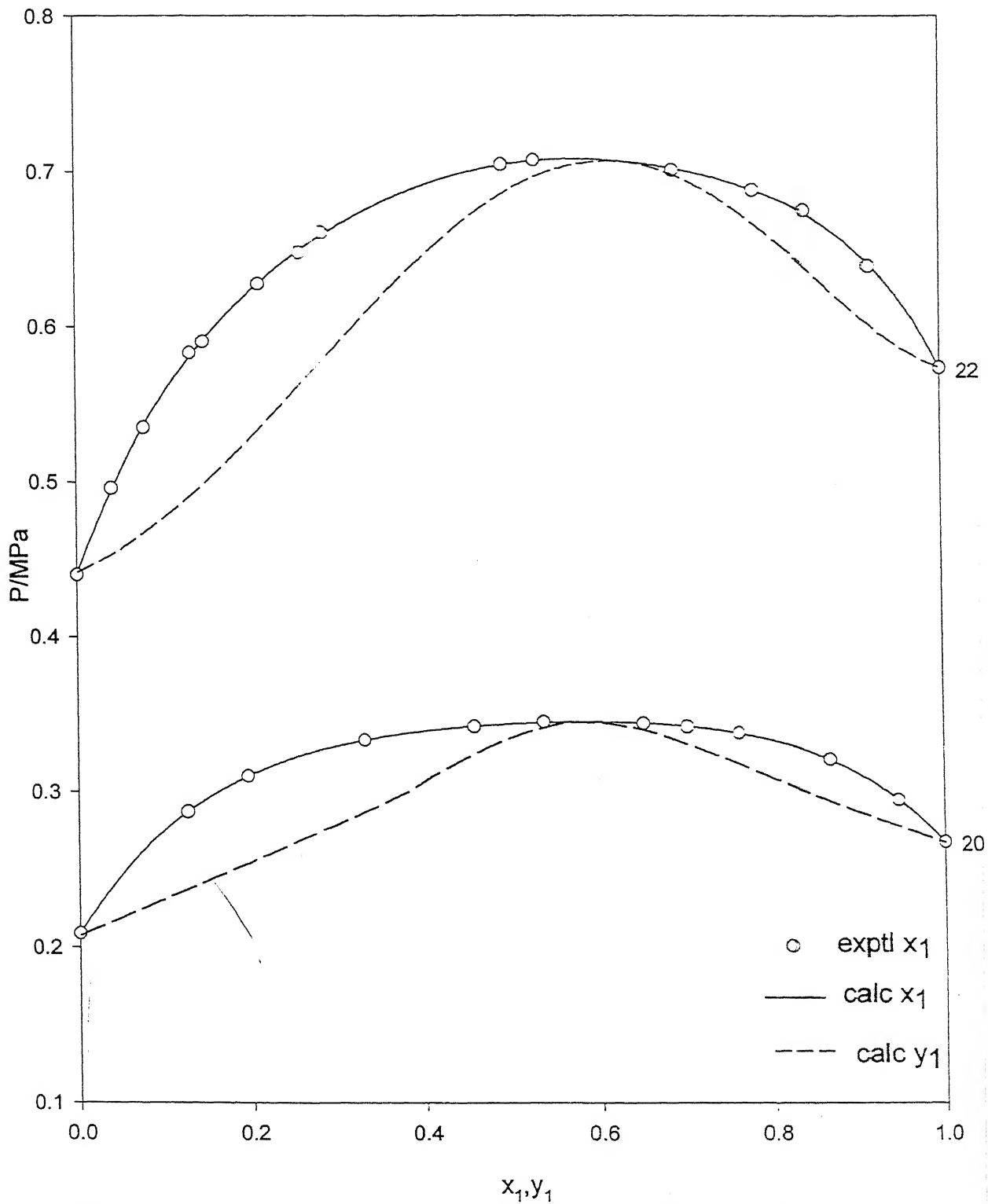


Fig. 4.6 Vapor-liquid equilibrium pressures and phase compositions for R-23(1)/R-116(2) mixtures at different temperatures (K).

Table 4.9: Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-134a(2) mixtures with different g^E models (contd.).

x ₁	y ₁				P(MPa)			
	exptl	calc			exptl	calc		
		NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
263.15 K								
0.000	0.000	0.000	0.000	0.200	0.201	0.201	0.201	0.201
0.225	0.451	0.435	0.433	0.289	0.278	0.291	0.291	0.291
0.392	0.618	0.644	0.612	0.345	0.345	0.345	0.345	0.345
0.700	0.854	0.866	0.853	0.468	0.468	0.453	0.453	0.453
1.000	1.000	1.000	1.000	0.58	0.58	0.579	0.579	0.579
	%AAD	1.833	0.917	%AAD	0.925	0.931	0.914	0.914
273.15 K								
0.000	0.000	0.000	0.000	0.292	0.293	0.293	0.293	0.293
0.233	0.432	0.433	0.435	0.408	0.407	0.409	0.409	0.409
0.384	0.600	0.611	0.611	0.485	0.485	0.485	0.485	0.485
0.710	0.847	0.858	0.858	0.654	0.656	0.651	0.651	0.651
1.000	1.000	1.000	1.000	0.811	0.808	0.808	0.808	0.808
	%AAD	0.626	0.719	%AAD	0.270	0.241	0.245	0.245

%AAD = average absolute deviation -- defined as $(\sum abs((exp - calc) / exp) * 100) / N$

Table 4.9: Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-134a(2) mixtures with different g^E models (contd.).

x ₁	y ₁			P(MPa)			
	exptl	calc		exptl	calc		
		NRTL	UNIQUAC		UNIQUAC-R	NRTL	UNIQUAC
283.15 K							
0.000	0.000	0.000	0.000	0.414	0.415	0.415	0.415
0.241	0.419	0.428	0.433	0.571	0.571	0.571	0.570
0.572	0.738	0.758	0.763	0.797	0.799	0.797	0.797
0.745	0.868	0.870	0.873	0.929	0.92	0.915	0.915
1.000	1.000	1.000	1.000	1.104	1.101	1.101	1.101
	%AAD	1.025	1.463	%AAD	0.337	0.405	0.418
293.15 K							
0.000	0.000	0.000	0.000	0.571	0.570	0.570	0.570
0.238	0.403	0.404	0.411	0.770	0.758	0.769	0.769
0.576	0.722	0.751	0.751	1.062	1.061	1.061	1.061
0.760	0.857	0.874	0.875	1.235	1.235	1.228	1.228
1.000	1.000	1.000	1.000	1.471	1.468	1.468	1.468
	%AAD	1.267	1.612	%AAD	0.411	0.234	0.213
303.15 K							
0.000	0.000	0.000	0.000	0.769	0.768	0.768	0.768
0.227	0.376	0.376	0.381	1.009	0.994	1.039	1.038
0.5646	0.7114	0.710	0.717	1.380	1.380	1.380	1.380
0.7541	0.8499	0.843	0.860	1.608	1.611	1.596	1.596
1.000	1.000	1.000	1.000	1.923	1.922	1.922	1.922
	%AAD	0.860	0.661	%AAD	0.350	0.773	0.778

%AAD = average absolute deviation - defined as $(\sum abs((exp - calc) / exp) * 100) / N$

Table 4.9: Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-134a(2) mixtures with different g^E models.

x_1	y_1		P(MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		NRTL	UNIQUAC
			UNIQUAC-R			UNIQUAC-R

313.15 K

0.000	0.000	0.000	0.000	1.015	1.015	1.015	1.015276
0.214	0.3409	0.346	0.350	1.289	1.289	1.332	1.331788
0.447	0.6077	0.612	0.600	1.625	1.618	1.625	1.624855
0.6709	0.7808	0.796	0.792	1.939	1.954	1.931	1.930366
1.000	1.000	1.000	1.000	2.475	2.476	2.476	2.475848
	%AAD	0.852	1.072	%AAD	0.266	0.769	0.776

323.15 K

0.000	0.000	0.000	0.000	1.316	1.318	1.318	1.318
0.2079	0.3209	0.323	0.325	1.643	1.638	1.685	1.684
0.4453	0.585	0.594	0.584	2.051	2.051	2.051	2.050
0.6742	0.7708	0.787	0.786	2.467	2.482	2.445	2.444
1.000	1.000	1.000	1.000	3.136	3.144	3.144	3.144
	%AAD	0.848	0.676	%AAD	0.249	0.770	0.775

%AAD = average absolute deviation -- defined as $(\sum abs((exp - calc) / exp) * 100) / N$

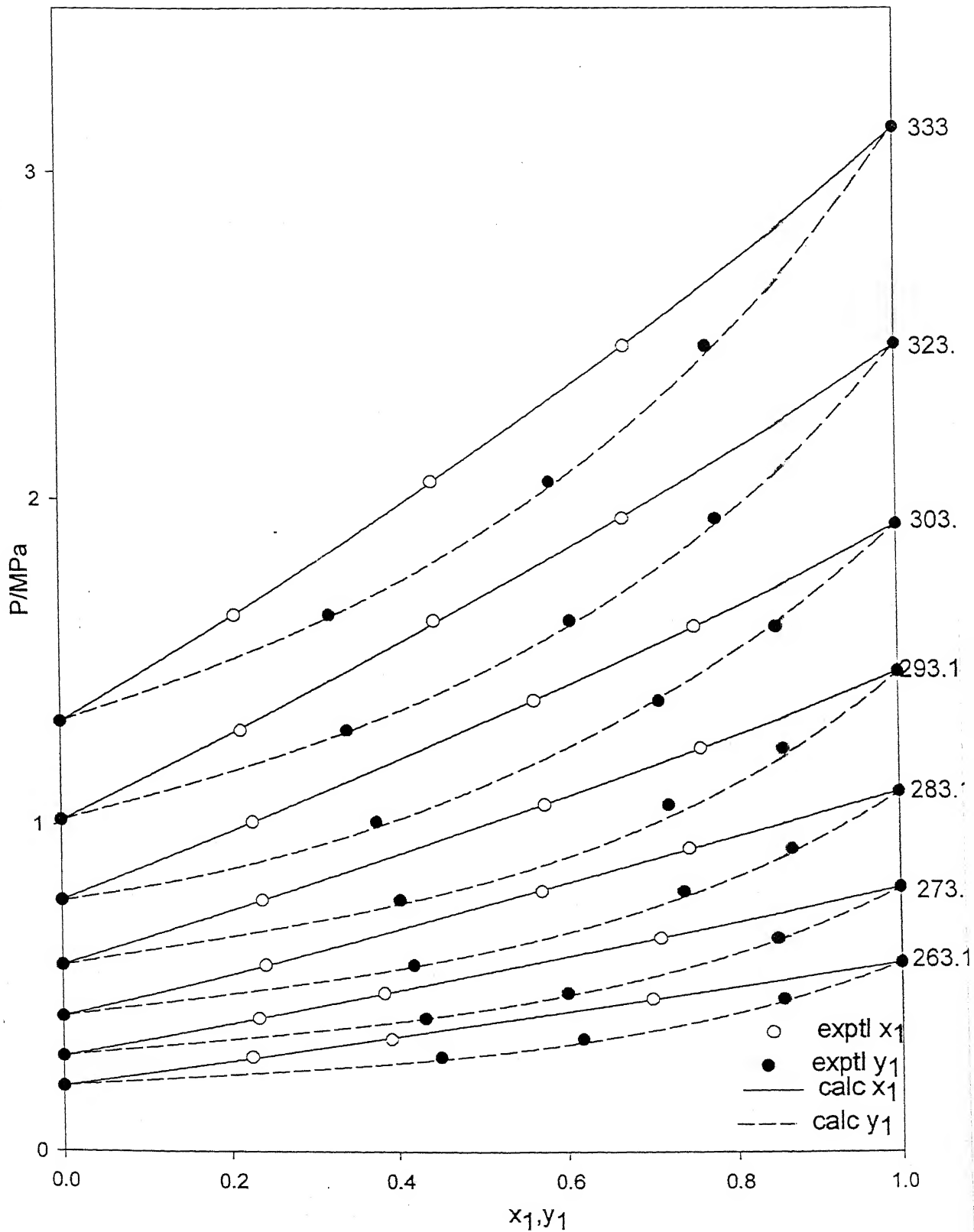


Fig. 4.8 Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-134a(2) mixtures at different temperatures (K).

Table 4.10: Vapor-liquid equilibrium pressures and phase compositions for R-125(1)/R-134a(2) mixtures with different g^E models (contd.).

x ₁	y ₁		P(MPa)				
	exptl	calc			exptl	calc	
		NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC
268.15 K							
0.000	0.000	0.000	0.000	0.000	0.241	0.240	0.242
0.032	0.070	0.069	0.071	0.071	0.254	0.253	0.254
0.153	0.275	0.288	0.285	0.285	0.293	0.293	0.293
0.296	0.468	0.485	0.477	0.477	0.338	0.341	0.338
0.463	0.672	0.655	0.650	0.650	0.405	0.396	0.392
0.778	0.866	0.878	0.880	0.880	0.494	0.497	0.494
0.926	0.963	0.961	0.962	0.962	0.544	0.544	0.543
1.000	1.000	1.000	1.000	1.000	0.567	0.565	0.564
	%AAD	2.424	1.969	1.959	%AAD	0.687	0.602
273.15 K							
0.000	0.000	0.000	0.000	0.000	0.291	0.291	0.291
0.038	0.077	0.079	0.081	0.081	0.308	0.306	0.307
0.126	0.225	0.239	0.241	0.241	0.341	0.34	0.341
0.256	0.414	0.428	0.427	0.427	0.39	0.39	0.391
0.381	0.557	0.570	0.568	0.568	0.438	0.438	0.438
0.519	0.693	0.695	0.694	0.694	0.492	0.49	0.490
0.661	0.795	0.800	0.800	0.800	0.542	0.543	0.543
0.784	0.879	0.878	0.879	0.879	0.591	0.588	0.588
0.896	0.944	0.943	0.943	0.943	0.633	0.629	0.629
1.000	1.000	1.000	1.000	1.000	0.672	0.671	0.672
	%AAD	2.023	2.324	2.326	%AAD	0.324	0.279

%AAD = average absolute deviation defined as $\left(\sum \text{abs}((\text{exp} - \text{calc})/\text{exp}) * 100 \right) / N$

Table 4.10: Vapor-liquid equilibrium pressures and phase compositions for R-125(1)/R-134a(2) mixtures with different g^E models (contd.).

x ₁	y ₁			P(MPa)		
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		UNIQUAC-R	NRTL
278.15 K						
0.000	0.000	0.000	0.000	0.331	0.291	0.291
0.153	0.27	0.276	0.274	0.415	0.415	0.427
0.392	0.561	0.573	0.550	0.516	0.520	0.516
0.602	0.755	0.753	0.745	0.611	0.611	0.602
0.784	0.873	0.875	0.876	0.689	0.688	0.682
1.000	1.000	1.000	1.000	0.785	0.784	0.783
	%AAD	1.236	1.319	%AAD	0.256	1.375
						1.726
283.15 K						
0.000	0.000	0.000	0.000	0.422	0.421	0.422
0.049	0.094	0.094	0.097	0.442	0.436	0.438
0.16	0.271	0.279	0.280	0.493	0.490	0.493
0.264	0.407	0.422	0.420	0.542	0.542	0.544
0.36	0.512	0.532	0.530	0.591	0.590	0.591
0.472	0.631	0.641	0.639	0.645	0.646	0.646
0.609	0.751	0.753	0.752	0.713	0.714	0.713
0.786	0.873	0.873	0.873	0.802	0.801	0.800
0.944	0.970	0.968	0.968	0.882	0.878	0.878
1.000	1.000	1.000	1.000	0.915	0.915	0.916
	%AAD	1.646	1.902	%AAD	0.381	0.273

%AAD) average absolute deviation defined as $(\sum abs((exp - calc)/(exp) * 100))/N$

Table 4.10: Vapor-liquid equilibrium pressures and phase compositions for R-125(1)/R-134a(2) mixtures with different g^E models.

x ₁	y ₁				P(MPa)			
	exptl	calc			exptl	calc		
		NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
293.15 K								
0.000	0.000	0.000	0.000	0.581	0.581	0.581	0.581	0.581
0.055	0.097	0.101	0.104	0.606	0.604	0.606	0.606	0.606
0.137	0.230	0.235	0.236	0.658	0.656	0.659	0.659	0.659
0.255	0.386	0.398	0.394	0.732	0.732	0.732	0.732	0.732
0.381	0.535	0.540	0.535	0.816	0.813	0.810	0.810	0.810
0.526	0.662	0.674	0.671	0.903	0.906	0.901	0.901	0.901
0.657	0.770	0.776	0.775	0.983	0.989	0.983	0.983	0.983
0.931	0.958	0.957	0.958	1.158	1.160	1.158	1.158	1.158
1.000	1.000	1.000	1.000	1.196	1.196	1.196	1.196	1.198
	%AAD	1.916	1.945	%AAD	0.303	0.150	0.150	0.150
			1.9446					

$$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$$

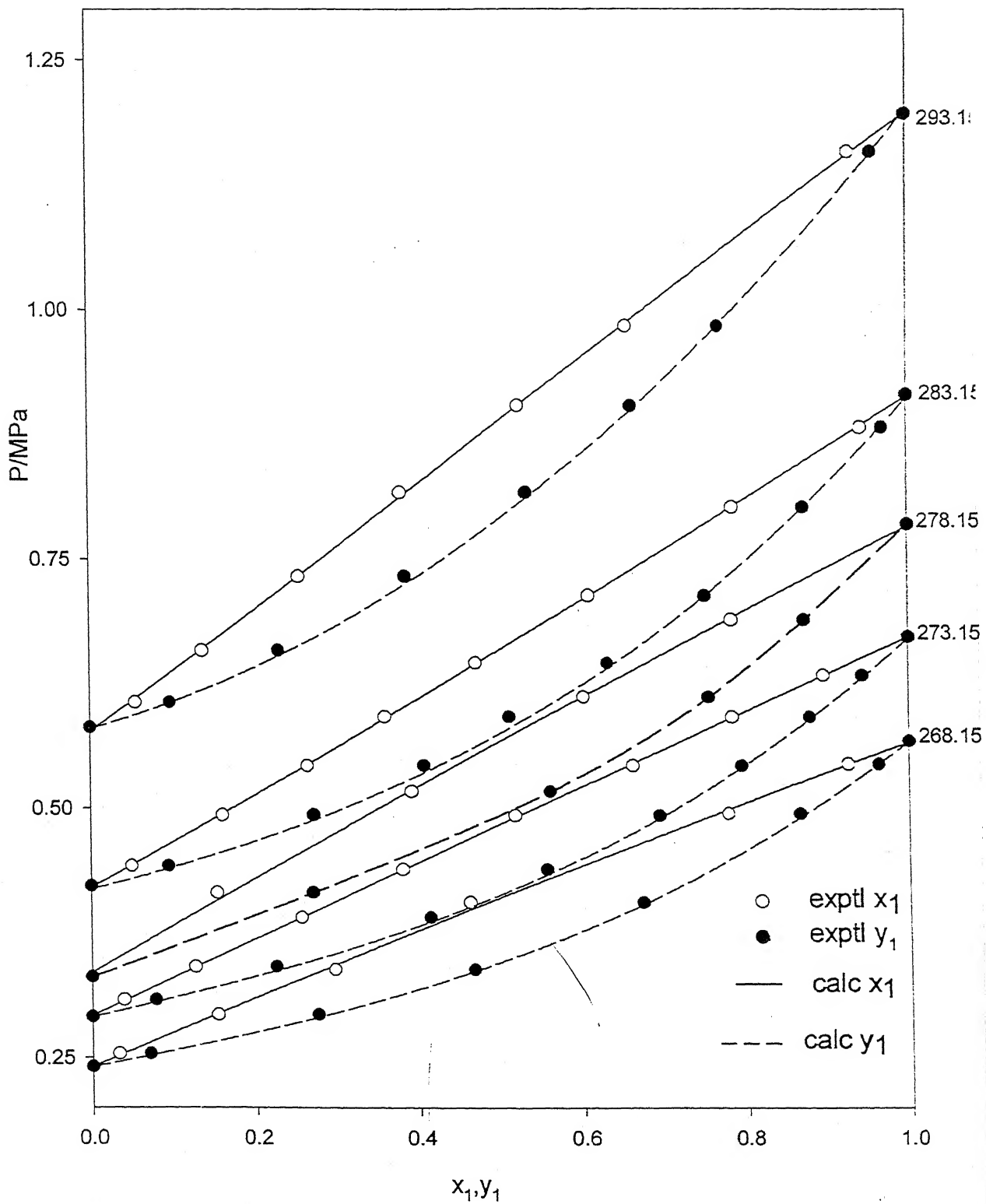


Fig. 4.9 Vapor-liquid equilibrium pressures and phase compositions for R-125(1)/R-134a(2) mixtures at different temperatures (K).

Table 4.11: Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-125(2) mixtures with different g^E models (contd.).

x ₁	y ₁				P(MPa)			
	exptl	calc			exptl	calc		
		NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
283.05 K								
0.000	0.000	0.000	0.000	0.000	0.905	0.904	0.904	0.904
0.241	0.283	0.292	0.285	0.286	0.992	0.998	1.017	1.018
0.457	0.500	0.503	0.483	0.484	1.058	1.058	1.058	1.058
0.710	0.735	0.725	0.719	0.720	1.102	1.098	1.079	1.080
0.895	0.897	0.893	0.899	0.900	1.125	1.105	1.090	1.090
1.000	1.000	1.000	1.000	1.000	1.104	1.098	1.098	1.098
	%AAD	0.923	1.107	1.106	%AAD	0.586	1.410	1.409
293.05 K								
0.000	0.000	0.000	0.000	0.000	1.202	1.201	1.201	1.201
0.241	0.279	0.286	0.279	0.280	1.310	1.318	1.344	1.345
0.453	0.493	0.497	0.477	0.478	1.395	1.395	1.395	1.396
0.709	0.732	0.726	0.721	0.721	1.456	1.453	1.427	1.427
0.896	0.897	0.896	0.903	0.903	1.480	1.468	1.448	1.448
1.000	1.000	1.000	1.000	1.000	1.472	1.464	1.464	1.464
	%AAD	0.702	0.921	0.922	%AAD	0.378	1.234	1.232

%AAD = average absolute deviation – defined as $(\sum \text{abs}(\text{exp} - \text{calc}) / \text{exp}) * 100 / N$

Table 4.11: Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-125(2) mixtures with different g^E models.

x_1	y_1		P(MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		NRTL	UNIQUAC
			UNIQUAC-R			UNIQUAC-R
303.05 K						
0.000	0.000	0.000	0.000	1.563	1.580	1.566
0.235	0.266	0.271	0.269	1.700	1.705	1.731
0.448	0.487	0.488	0.474	1.801	1.801	1.802
0.708	0.728	0.729	0.723	1.894	1.888	1.854
0.895	0.896	0.900	0.903	1.923	1.925	1.890
1.000	1.000	1.000	1.000	1.922	1.935	1.917
	%AAD	0.439	0.907	%AAD	0.418	1.015
313.05 K						
0.000	0.000	0.000	0.000	2.001	2.010	2.010
0.225	0.257	0.257	0.254	2.167	2.172	2.214
0.448	0.478	0.485	0.470	2.306	2.306	2.308
1.000	1.000	1.000	1.000	2.477	2.471	2.471
	%AAD	0.371	0.766	%AAD	0.238	0.710

$\%AAD = \text{average absolute deviation} - \text{defined as } (\sum abs((exp - calc) / exp) * 100) / N$

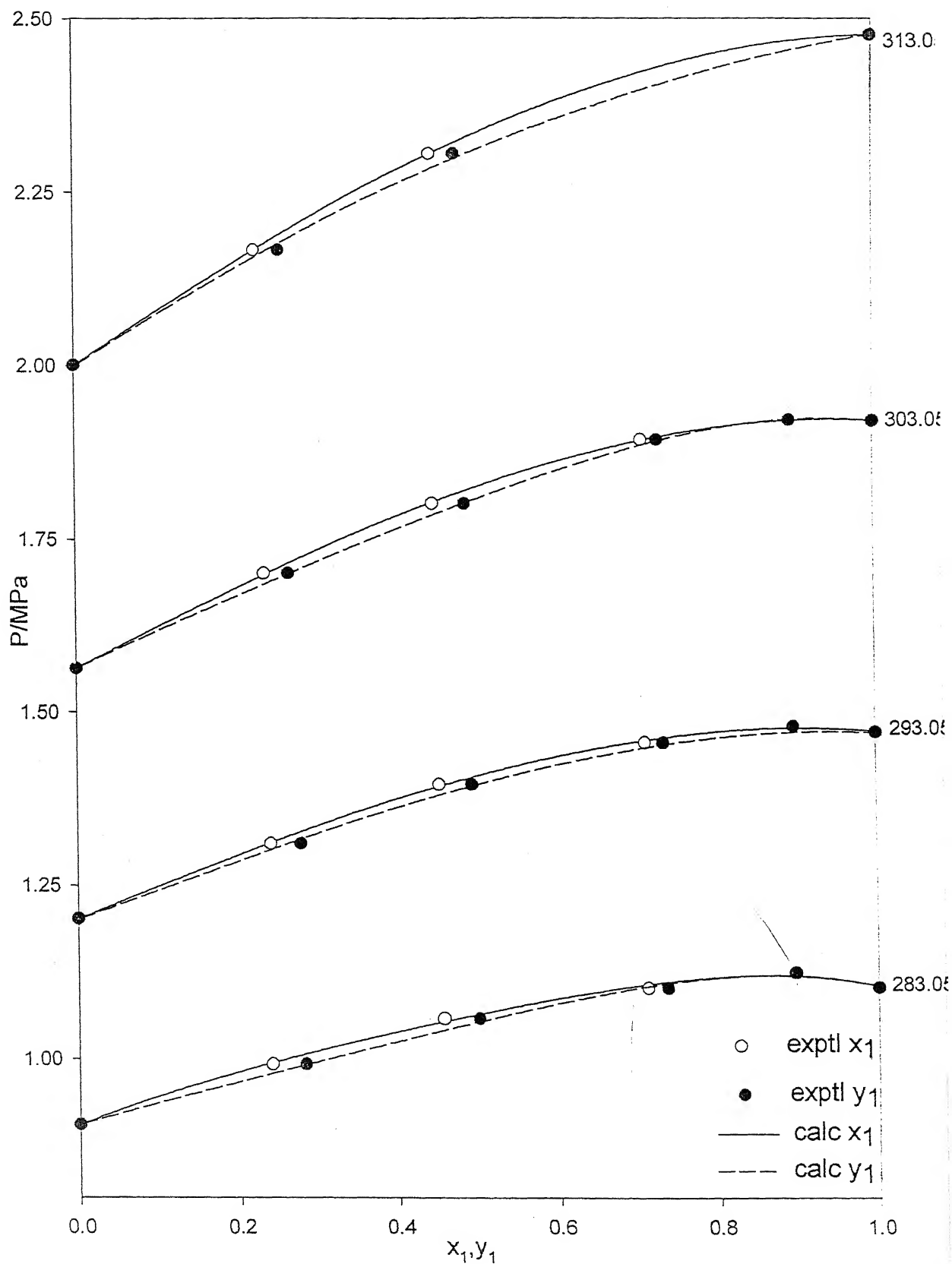


Fig. 4.10 Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-125(2) mixtures at different temperatures (K).

Table 4.12: Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-12(2) mixtures with different g^E models.

x_1	y_1		P(MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		NRTL	UNIQUAC
			UNIQUAC-R			UNIQUAC-R
343.81 K						
0.000	0.000	0.000	0.000	1.869	1.877	1.865
0.036	0.057	0.059	0.059	1.947	1.953	1.953
0.088	0.132	0.133	0.133	2.026	2.050	2.050
0.172	0.243	0.236	0.236	2.178	2.184	2.184
0.223	0.301	0.293	0.293	2.252	2.257	2.257
0.286	0.371	0.359	0.359	2.341	2.341	2.341
0.327	0.414	0.400	0.400	2.405	2.392	2.392
0.393	0.481	0.464	0.464	2.479	2.471	2.471
0.498	0.574	0.562	0.562	2.612	2.588	2.588
0.575	0.683	0.631	0.631	2.675	2.668	2.668
0.708	0.750	0.748	0.748	2.798	2.797	2.797
0.739	0.776	0.775	0.775	2.818	2.826	2.826
0.772	0.802	0.803	0.803	2.853	2.855	2.855
0.793	0.820	0.821	0.821	2.872	2.874	2.874
0.866	0.881	0.884	0.884	2.916	2.937	2.937
0.917	0.925	0.928	0.928	2.951	2.979	2.979
0.942	0.947	0.950	0.950	2.970	2.999	2.999
1.000	1.000	1.000	1.000	3.010	3.045	3.045
	%AAD	2.686	1.726	%AAD	0.483	0.472

$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$

Table 4.13: Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-123(2) mixtures with different g^E models (contd.).

x ₁	y ₁		P(MPa)				
	exptl	calc		exptl	calc		
		NRTL	UNIQUAC		UNIQUAC-R	NRTL	UNIQUAC
414.57 K							
0.000	0.000	0.000	0.000	0.000	1.785	1.795	1.784
0.034	0.053	0.080	0.091	0.091	1.883	1.949	1.981
0.079	0.168	0.175	0.187	0.186	2.158	2.164	2.238
0.184	0.325	0.350	0.347	0.348	2.687	2.713	2.814
0.221	0.375	0.400	0.391	0.391	2.922	2.922	3.022
0.257	0.411	0.443	0.429	0.428	3.104	3.131	3.226
0.286	0.458	0.475	0.457	0.456	3.393	3.305	3.387
0.363	0.501	0.547	0.520	0.520	3.751	3.784	3.810
0.393	0.533	0.571	0.542	0.542	4.006	3.978	4.001
0.468	0.583	0.622	0.588	0.588	4.501	4.472	4.458
0.495	0.593	0.637	0.601	0.601	4.653	4.652	4.649
0.550	0.599	0.663	0.645	0.644	4.884	5.018	4.889
0.579	0.595	0.673	0.630	0.620	5.183	5.207	5.089
	%AAD	10.471	9.2	9.016	%AAD	0.098	2.205
							1.987

%AAD = average absolute deviation – defined as $(\sum abs((exp - calc)/exp) * 100) / N$

Table 4.13: Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-123(2) mixtures with different g^E models (contd.).

x ₁	y ₁				P(MPa)			
	exptl	calc			exptl	calc		
		NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
353.92 K								
0.000	0.000	0.000	0.000	0.490	0.516	0.516	0.510	
0.069	0.260	0.247	0.260	0.657	0.662	0.678	0.678	
0.237	0.575	0.589	0.585	1.040	1.083	1.078	1.077	
0.268	0.623	0.629	0.625	1.192	1.170	1.162	1.160	
0.341	0.698	0.706	0.705	1.407	1.383	1.372	1.369	
0.425	0.754	0.772	0.775	1.569	1.643	1.635	1.631	
0.474	0.784	0.803	0.808	1.800	1.800	1.797	1.792	
0.496	0.812	0.816	0.821	1.898	1.872	1.872	1.866	
0.584	0.838	0.858	0.865	2.094	2.162	2.176	2.169	
0.632	0.868	0.878	0.885	2.319	2.324	2.344	2.337	
0.659	0.879	0.888	0.894	2.412	2.415	2.439	2.431	
0.719	0.903	0.908	0.914	2.647	2.621	2.648	2.640	
0.789	0.929	0.930	0.935	2.912	2.865	2.891	2.884	
0.873	0.956	0.955	0.958	3.216	3.173	3.189	3.185	
1.000	1.000	1.000	1.000	3.725	3.725	3.721	3.722	
	%AAD	1.440	1.347	%AAD	1.953	2.191	1.955	

%AAD = average absolute deviation defined as $(\sum \text{abs}((\text{exp} - \text{calc})/\text{exp}) * 100) / N$

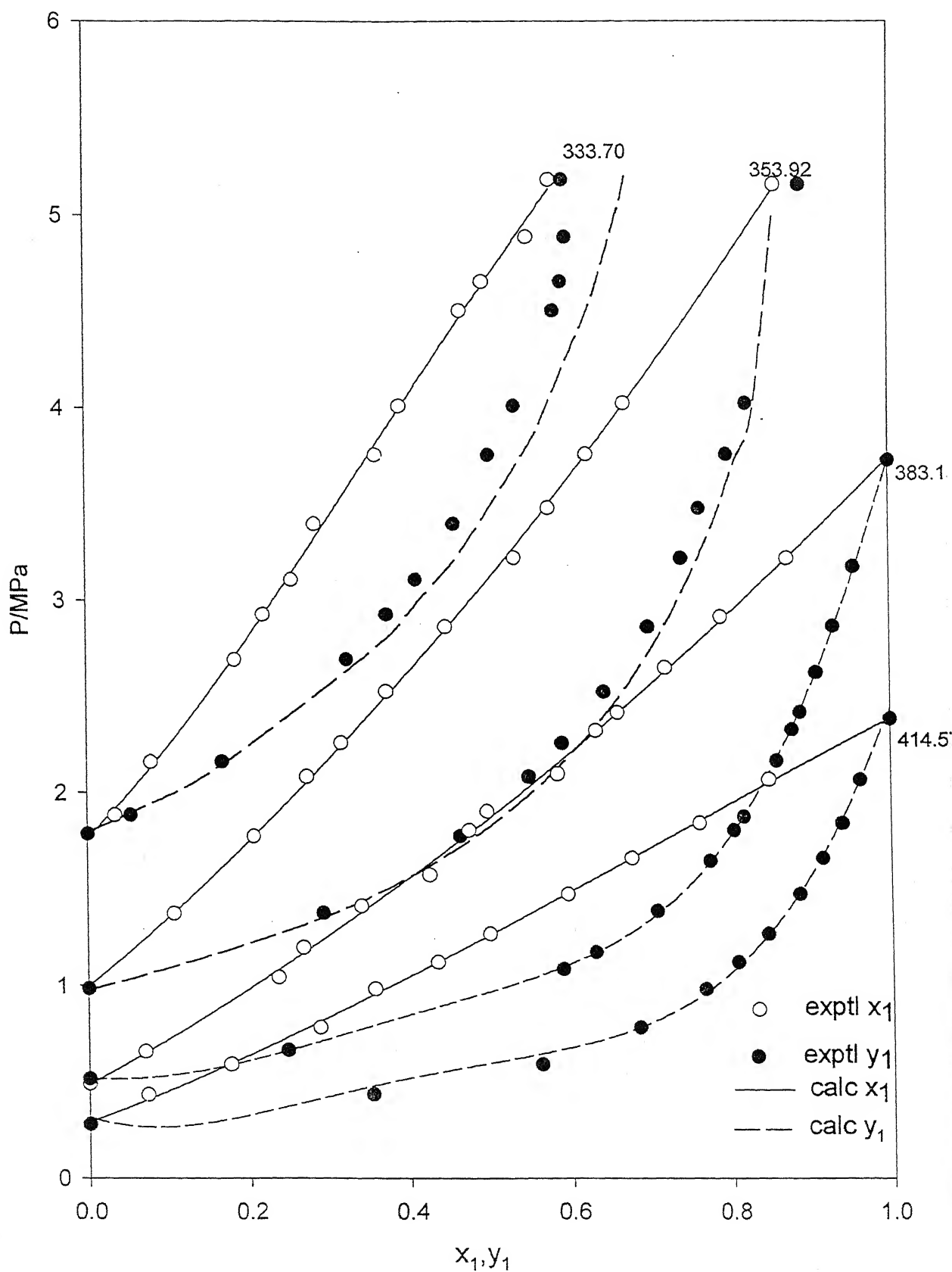


Fig. 4.11 Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-123(2) mixtures at different temperatures (K).

Table 4.13: Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-123(2) mixtures with different g^E models.

x_1	y_1		P (MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		NRTL	UNIQUAC
			UNIQUAC-R			UNIQUAC-R
333.7 K						
0.000	0.000	0.000	0.000	0.279	0.313	0.313
0.072	0.354	0.291	0.302	0.432	0.423	0.432
0.176	0.561	0.538	0.535	0.588	0.600	0.601
0.288	0.683	0.692	0.686	0.780	0.813	0.802
0.357	0.765	0.756	0.752	0.980	0.954	0.939
0.434	0.807	0.810	0.808	1.118	1.118	1.101
0.498	0.845	0.845	0.846	1.265	1.258	1.243
0.596	0.885	0.888	0.890	1.471	1.477	1.469
0.675	0.914	0.915	0.917	1.657	1.657	1.654
0.760	0.939	0.939	0.942	1.839	1.853	1.853
0.848	0.962	0.961	0.963	2.064	2.061	2.062
1.000	1.000	1.000	1.000	2.381	2.460	2.460
	%AAD	2.105	1.939	%AAD	2.384	2.447

$$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$$

Table 4.14: Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-124(2) mixtures with different g^E models (contd.-).

x_1	y_1		P(MPa)			
	exptl	NRTL	calc		exptl	NRTL
			UNIQUAC	UNIQUAC-R		
296.45 K						
0.000	0.000	0.000	0.000	0.000	3.700	3.618
0.193	0.297	0.295	0.293	0.293	4.210	4.220
0.409	0.542	0.538	0.532	0.532	4.850	4.850
0.558	0.663	0.672	0.668	0.668	5.270	5.251
0.755	0.835	0.825	0.825	0.825	5.720	5.741
1.000	1.000	1.000	1.000	1.000	6.210	6.296
	%AAD	0.681	0.883	0.88	%AAD	0.758
						0.89
						0.8903
302.25 K						
0.000	0.000	0.000	0.000	0.000	4.310	4.321
0.102	0.171	0.171	0.171	0.171	4.730	4.739
0.180	0.286	0.281	0.280	0.280	5.060	5.043
0.237	0.354	0.352	0.351	0.351	5.260	5.257
0.368	0.488	0.496	0.495	0.495	5.720	5.720
0.678	0.766	0.762	0.763	0.763	6.670	6.670
0.761	0.825	0.824	0.825	0.825	6.880	6.893
0.865	0.901	0.900	0.901	0.901	7.160	7.158
1.000	1.000	1.000	1.000	1.000	7.480	7.476
	%AAD	0.553	0.587	0.590	%AAD	0.125
						0.143
						0.141

$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \frac{\text{abs}(\text{exp} - \text{calc})}{\text{exp}} \right) * 100 / N$

Table 4.15: Vapor-liquid equilibrium pressures and phase compositions for R-124a(1)/R-142b(2) mixtures with different g^E models (contd.).

x_1	y_1		P(MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC	UNIQUAC-R	NRTL	UNIQUAC
298.15 K						
0.000	0.000	0.000	0.000	0.000	3.380	3.384
0.039	0.041	0.041	0.041	0.041	3.390	3.394
0.050	0.053	0.052	0.053	0.053	3.390	3.397
0.189	0.196	0.200	0.199	0.199	3.430	3.429
0.240	0.263	0.255	0.253	0.253	3.450	3.443
0.431	0.452	0.458	0.457	0.457	3.510	3.511
0.540	0.566	0.570	0.570	0.570	3.560	3.560
0.587	0.611	0.617	0.617	0.617	3.590	3.583
0.684	0.703	0.712	0.712	0.712	3.620	3.634
0.783	0.800	0.806	0.806	0.806	3.690	3.688
0.947	0.949	0.954	0.954	0.954	3.770	3.783
1.000	1.000	1.000	1.000	1.000	3.790	3.815
	%AAD	1.129	0.964	0.964	%AAD	0.194
					0.198	0.193

$$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$$

Table 4.15: Vapor-liquid equilibrium pressures and phase compositions for R-124a(1)/R-142b(2) mixtures with different g^E models.

x ₁	y ₁		P(MPa)				
	exptl	calc		exptl	calc		
		NRTL	UNIQUAC		UNIQUAC-R	NRTL	UNIQUAC
312.15 K							
0.000	0.000	0.000	0.000	0.000	5.080	5.104	5.104
0.035	0.037	0.036	0.038	0.038	5.100	5.111	5.122
0.124	0.134	0.132	0.130	0.130	5.140	5.140	5.157
0.240	0.257	0.257	0.252	0.252	5.200	5.197	5.199
0.329	0.346	0.352	0.347	0.347	5.260	5.249	5.238
0.508	0.536	0.534	0.535	0.535	5.360	5.358	5.344
0.664	0.692	0.688	0.692	0.692	5.460	5.458	5.460
0.770	0.792	0.791	0.793	0.793	5.530	5.534	5.548
0.791	0.817	0.811	0.813	0.813	5.550	5.550	5.566
0.867	0.890	0.883	0.883	0.883	5.610	5.616	5.633
1.000	1.000	1.000	1.000	1.000	5.730	5.755	5.755
	%AAD	0.685	0.771	0.772	%AAD	0.149	0.313

$$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$$

Table 4.16: Vapor-liquid equilibrium pressures and phase compositions for R-142b(1)/R-141b(2) at 324.4 K with different g^E models.

x_1	y_1		P(MPa)			
	exptl	NRTL	calc		exptl	NRTL
			UNIQUAC	UNIQUAC-R		
0.000	0.000	0.000	0.000	0.000	0.185	0.182
0.092	0.262	0.277	0.278	0.278	0.234	0.232
0.188	0.444	0.460	0.459	0.459	0.283	0.283
0.287	0.573	0.591	0.589	0.589	0.333	0.335
0.388	0.669	0.688	0.686	0.686	0.383	0.386
0.463	0.730	0.745	0.743	0.743	0.417	0.423
0.490	0.749	0.763	0.762	0.762	0.433	0.436
0.593	0.814	0.824	0.824	0.824	0.484	0.486
0.697	0.870	0.876	0.876	0.876	0.535	0.534
0.682	0.864	0.869	0.869	0.869	0.526	0.527
0.792	0.917	0.918	0.918	0.918	0.582	0.579
0.899	0.958	0.961	0.961	0.961	0.635	0.630
1.000	1.000	1.000	1.000	1.000	0.685	0.679
	%AAD	1.721	1.657	1.648	%AAD	0.689
						4.905
						0.182
						0.233
						0.283
						0.334
						0.385
						0.434
						0.484
						0.533
						0.421
						0.526
						0.578
						0.629
						0.679
						4.040

%AAD = average absolute deviation – defined as $(\sum abs((exp - calc) / exp) * 100) / N$

Table 4.17: Vapor-liquid equilibrium pressures and phase compositions for R-142b(1)/R-140a(2) mixtures at 323.4 K with different g^E models.

x ₁	y ₁				P(MPa)			
	exptl	calc		exptl	calc			
		NRTL	UNIQUAC		UNIQUAC-R	NRTL	UNIQUAC	UNIQUAC-R
0.000	0.000	0.000	0.000	0.047	0.043	0.043	0.044	
0.088	0.650	0.653	0.659	0.119	0.117	0.119	0.119	
0.177	0.797	0.796	0.798	0.186	0.186	0.187	0.188	
0.266	0.866	0.860	0.860	0.253	0.249	0.250	0.251	
0.371	0.903	0.900	0.900	0.317	0.317	0.317	0.317	
0.435	0.922	0.917	0.917	0.353	0.356	0.356	0.355	
0.481	0.931	0.927	0.927	0.383	0.383	0.383	0.383	
0.583	0.951	0.945	0.945	0.440	0.440	0.440	0.440	
0.666	0.964	0.957	0.957	0.484	0.485	0.486	0.485	
0.735	0.970	0.966	0.966	0.524	0.522	0.523	0.524	
0.785	0.976	0.972	0.973	0.552	0.549	0.550	0.551	
0.897	0.989	0.986	0.986	0.620	0.613	0.613	0.614	
1.000	1.000	1.000	1.000	0.685	0.679	0.679	0.679	
	%AAD	0.398	0.466	%AAD	1.240	0.996	0.883	

$$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$$

R-142b(1)/R-140a(2) at 324.40 K

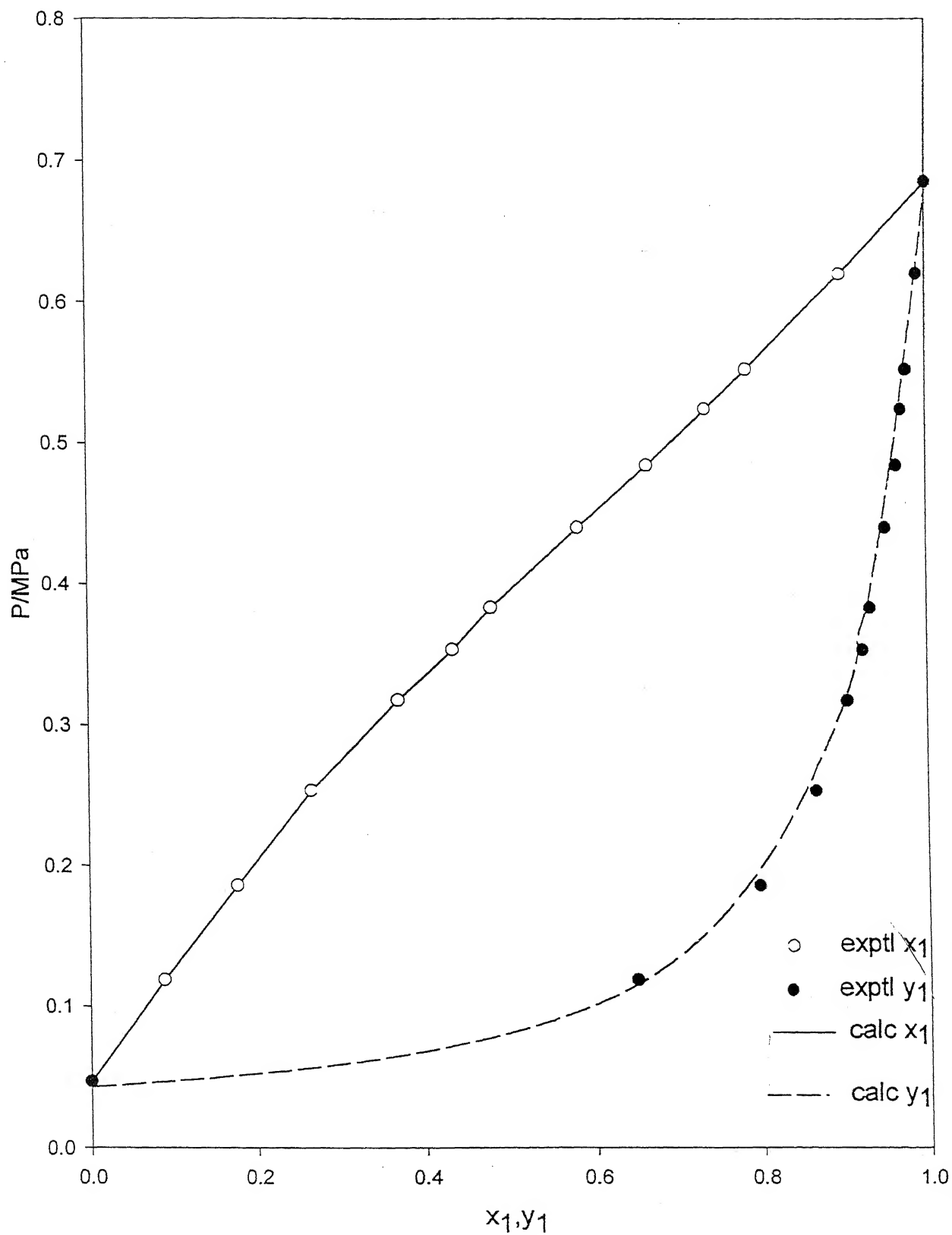


Fig. 4.12 Vapor-liquid equilibrium pressures and phase compositions for R-142b(2)/R-140a(2) mixtures at 323.40 K.

Table 4.18: Vapor-liquid equilibrium pressures and phase compositions for R-141b(1)/R-140a(2) mixtures at 323.4 K with different g^E models.

x ₁	y ₁				P(MPa)			
	exptl	calc			exptl	calc		
		NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
0.000	0.000	0.000	0.000	0.047	0.043	0.043	0.044	
0.097	0.311	0.340	0.333	0.062	0.059	0.059	0.059	
0.195	0.502	0.529	0.527	0.076	0.075	0.074	0.074	
0.280	0.626	0.636	0.638	0.087	0.088	0.087	0.087	
0.396	0.733	0.738	0.742	0.104	0.104	0.104	0.104	
0.489	0.804	0.798	0.807	0.117	0.117	0.118	0.118	
0.497	0.805	0.802	0.802	0.131	0.131	0.132	0.131	
0.599	0.858	0.853	0.857	0.145	0.144	0.144	0.144	
0.694	0.910	0.894	0.898	0.158	0.156	0.157	0.152	
0.699	0.903	0.896	0.896	0.116	0.117	0.117	0.115	
0.798	0.940	0.932	0.934	0.146	0.143	0.144	0.145	
0.800	0.942	0.933	0.933	0.156	0.156	0.156	0.156	
0.900	0.974	0.967	0.967	0.172	0.169	0.169	0.169	
1.000	1.000	1.000	1.000	0.185	0.182	0.182	0.183	
	%AAD	1.707	1.448	%AAD	1.569	1.691	1.778	

$AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$

Table 4.19: Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-22(2) mixtures at 283.0 K with different g^E models.

x_1	y_1				P(MPa)			
	exptl	calc			exptl	calc		
		NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
0.000	0.000	0.000	0.000	0.000	0.677	0.675	0.675	0.675
0.114	0.168	0.171	0.173	0.173	0.733	0.729	0.731	0.731
0.208	0.292	0.295	0.299	0.299	0.777	0.774	0.777	0.777
0.299	0.399	0.403	0.408	0.408	0.820	0.817	0.821	0.821
0.406	0.511	0.516	0.520	0.520	0.867	0.866	0.869	0.869
0.503	0.604	0.608	0.610	0.610	0.908	0.908	0.910	0.910
0.602	0.692	0.694	0.695	0.694	0.950	0.950	0.950	0.950
0.703	0.772	0.776	0.776	0.775	0.990	0.990	0.988	0.988
0.504	0.605	0.609	0.612	0.611	0.904	0.909	0.911	0.911
0.702	0.787	0.776	0.776	0.775	0.989	0.990	0.988	0.988
0.800	0.851	0.851	0.851	0.851	1.026	1.028	1.024	1.024
0.901	0.928	0.927	0.928	0.928	1.065	1.065	1.062	1.062
1.000	1.000	1.000	1.000	1.000	1.104	1.101	1.101	1.101
	%AAD	0.658	1.089	1.089	%AAD	0.206	0.228	0.227

$\%AAD = \text{average absolute deviation} - \text{defined as } (\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100) / N$

Table 4.20: Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-12(2) mixtures at 283.0 K with different g^E models.

x_1	y_1				P(MPa)			
	exptl	calc		UNIQUAC-R	exptl	calc		
		NRTL	UNIQUAC			NRTL	UNIQUAC	UNIQUAC-R
0	0.000	0.000	0.000	0.000	0.420	0.420	0.420	0.420
0.0805	0.326	0.336	0.345	0.344	0.613	0.621	0.626	0.625
0.1802	0.502	0.491	0.503	0.500	0.783	0.782	0.787	0.784
0.2828	0.591	0.573	0.588	0.586	0.898	0.890	0.898	0.894
0.3884	0.654	0.630	0.648	0.645	0.983	0.969	0.979	0.976
0.4963	0.700	0.679	0.695	0.693	1.039	1.031	1.039	1.038
0.6004	0.739	0.725	0.736	0.735	1.081	1.078	1.082	1.082
0.7017	0.778	0.771	0.777	0.777	1.112	1.112	1.113	1.114
0.7792	0.814	0.811	0.813	0.813	1.123	1.130	1.129	1.130
0.8583	0.863	0.859	0.859	0.860	1.136	1.137	1.136	1.136
0.8937	0.891	0.885	0.885	0.886	1.134	1.136	1.134	1.135
0.9155	0.907	0.904	0.904	0.904	1.131	1.133	1.132	1.132
0.9368	0.926	0.923	0.924	0.924	1.127	1.128	1.127	1.127
0.9577	0.947	0.945	0.946	0.946	1.120	1.122	1.121	1.121
0.9718	0.963	0.962	0.962	0.962	1.116	1.116	1.115	1.115
1	1.000	1.000	1.000	1.000	1.104	1.100	1.100	1.100
	%AAD	1.240	0.633	0.631	%AAD	0.390	0.278	0.277

$\%AAD = \text{average absolute deviation} - \text{defined as } (\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100) / N$

R-32(1)/R-12(2) at 283.0 K

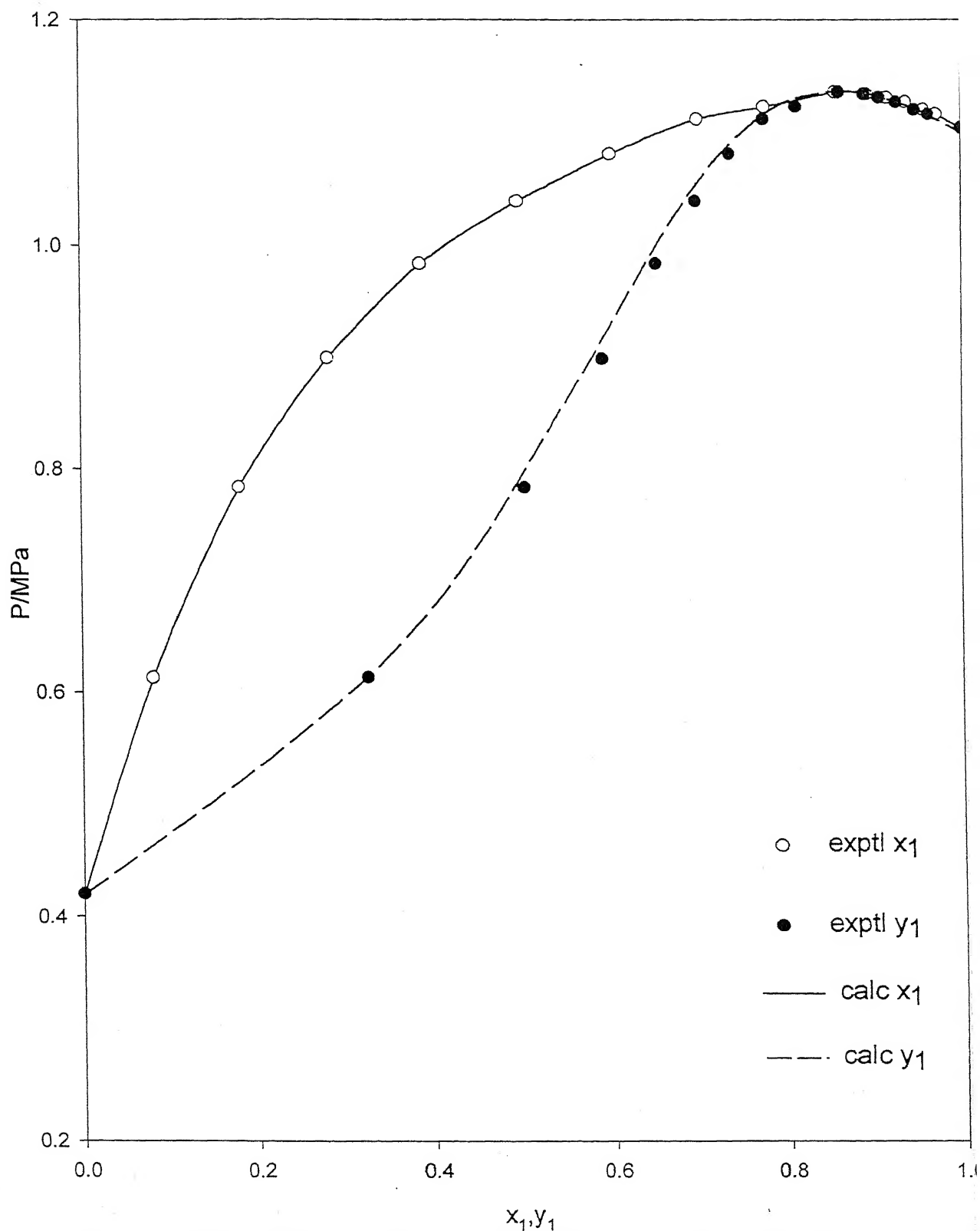


Fig. 4.13 Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-12(2) mixtures at 283.00 K.

Table 4.21: Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-40(2) mixtures at 283.0 K with different g^E models.

x_1	y_1			P(MPa)			
	exptl	calc		exptl	calc		
		NRTL	UNIQUAC		NRTL	UNIQUAC	UNIQUAC-R
0.000	0.000	0.000	0.000	0.362	0.362	0.362	0.362
0.098	0.324	0.319	0.327	0.505	0.494	0.500	0.500
0.191	0.481	0.479	0.484	0.605	0.599	0.605	0.605
0.300	0.597	0.596	0.598	0.704	0.700	0.704	0.704
0.399	0.669	0.669	0.671	0.777	0.776	0.778	0.778
0.500	0.731	0.730	0.730	0.844	0.844	0.844	0.843
0.600	0.785	0.782	0.782	0.901	0.903	0.901	0.901
0.700	0.834	0.831	0.832	0.956	0.957	0.955	0.954
0.802	0.887	0.883	0.883	1.008	1.009	1.006	1.006
0.901	0.940	0.937	0.938	1.055	1.056	1.054	1.054
1.000	1.000	1.000	1.000	1.104	1.100	1.100	1.100
	%AAD	0.319	0.278	%AAD	0.405	0.191	0.190

%AAD = average absolute deviation – defined as $(\sum abs((exp - calc) / exp) * 100) / N$

Table 4.22: Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)R-141b(2) mixtures with different g^E models (contd.).

x_1	y_1		P(MPa)			
	exptl	NRTL	calc		exptl	NRTL
			UNIQUAC	UNIQUAC-R		
278.15 K						
0.000	0.000	0.001	0.000	0.000	0.035	0.035
0.168	0.647	0.722	0.737	0.737	0.101	0.101
0.221	0.759	0.791	0.792	0.792	0.132	0.128
0.308	0.819	0.859	0.851	0.850	0.167	0.165
0.443	0.877	0.912	0.902	0.901	0.213	0.219
0.674	0.925	0.949	0.945	0.945	0.269	0.271
1.000	1.000	1.000	1.000	1.000	0.348	0.348
	%AAD	5.469	5.425	4.501	%AAD	1.790
						2.080
						1.786
288.15 K						
0.000	0.000	0.001	0.000	0.000	0.053	0.053
0.069	0.498	0.432	0.518	0.518	0.101	0.086
0.152	0.655	0.665	0.702	0.702	0.154	0.132
0.258	0.768	0.804	0.803	0.803	0.215	0.197
0.384	0.834	0.880	0.865	0.864	0.270	0.270
0.482	0.857	0.911	0.895	0.894	0.306	0.318
0.718	0.911	0.950	0.943	0.942	0.389	0.396
1.000	1.000	1.000	1.000	1.000	0.486	0.489
	%AAD	5.894	4.548	4.515	%AAD	5.403
						0.638
						0.452

%AAD = average absolute deviation – defined as $(\sum abs((exp - calc) / exp) * 100) / N$

Table 4.22: Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)R-141b(2) mixtures with different g^E models (contd.).

x ₁	y ₁				P(MPa)			
	exptl	calc		exptl	calc			
		NRTL	UNIQUAC		UNIQUAC-R	NRTL	UNIQUAC	UNIQUAC-R
318.15 K								
0.000	0.000	0.000	0.000	0.156	0.154	0.154	0.154	
0.041	0.215	0.295	0.300	0.221	0.215	0.217	0.217	
0.128	0.504	0.568	0.571	0.336	0.333	0.335	0.335	
0.208	0.624	0.684	0.686	0.431	0.431	0.432	0.431	
0.302	0.708	0.764	0.766	0.534	0.535	0.534	0.533	
0.407	0.785	0.820	0.822	0.638	0.638	0.638	0.637	
0.590	0.859	0.884	0.887	0.800	0.799	0.799	0.798	
0.809	0.925	0.944	0.946	0.999	0.981	0.981	0.980	
1.000	1.000	1.000	1.000	1.158	1.157	1.156	1.155	
	%AAD	10.948	11.595	%AAD	0.781	0.604	0.669	

$$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}(\text{exp} - \text{calc}) / \text{exp} \right) * 100 / N$$

Table 4.22: Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)R-141b(2) mixtures with different g^E models.

x_1	y_1		P(MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		NRTL	UNIQUAC
			UNIQUAC-R			UNIQUAC-R
333.15 K						
0.000	0.000	0.000	0.000	0.246	0.245	0.245
0.056	0.278	0.320	0.325	0.340	0.354	0.356
0.117	0.479	0.500	0.503	0.461	0.464	0.468
0.164	0.576	0.587	0.589	0.550	0.546	0.550
0.226	0.643	0.667	0.667	0.649	0.649	0.653
0.311	0.712	0.741	0.740	0.785	0.780	0.782
0.390	0.769	0.789	0.787	0.883	0.894	0.896
0.450	0.793	0.817	0.815	0.975	0.976	0.974
0.520	0.822	0.846	0.843	1.066	1.067	1.064
0.657	0.878	0.891	0.889	1.236	1.236	1.232
0.777	0.917	0.926	0.925	1.389	1.382	1.379
0.857	0.944	0.950	0.950	1.504	1.483	1.481
1.000	1.000	1.000	1.000	1.685	1.684	1.680
	%AAD	3.731	3.849	%AAD	0.874	1.016

$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$

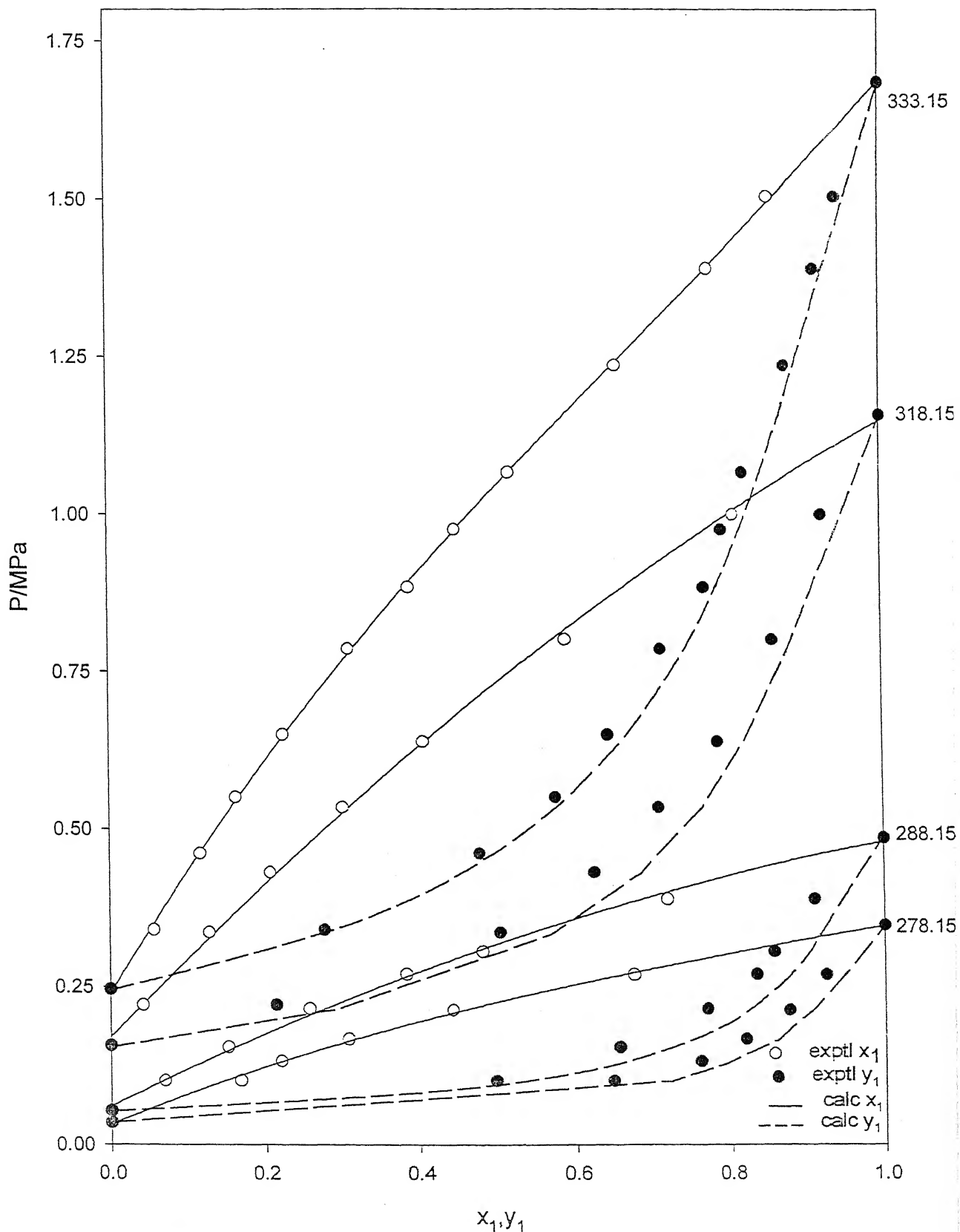


Fig. 4.14 Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-141b(2) mixtures at different temperatures (K).

Table 4.23: Vapor-liquid equilibrium pressures and phase compositions for R-23(1)/R-13(2) mixtures with different g^E models (contd.).

x ₁	y ₁		P (MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		UNIQUAC-R	UNIQUAC-R
272.94 K						
0.000	0.000	0.000	0.000	1.967	1.949	1.922
0.062	0.098	0.100	0.107	2.135	2.119	2.090
0.124	0.189	0.185	0.199	2.279	2.241	2.235
0.202	0.278	0.274	0.298	2.423	2.389	2.390
0.277	0.348	0.348	0.378	2.529	2.507	2.510
0.365	0.436	0.425	0.455	2.625	2.619	2.614
0.462	0.506	0.504	0.521	2.694	2.709	2.682
0.538	0.564	0.562	0.564	2.733	2.753	2.708
0.564	0.586	0.582	0.579	2.749	2.763	2.712
0.582	0.598	0.596	0.589	2.752	2.768	2.714
0.652	0.652	0.648	0.630	2.762	2.774	2.709
0.737	0.724	0.713	0.690	2.751	2.751	2.675
0.806	0.783	0.769	0.752	2.723	2.704	2.618
0.860	0.836	0.818	0.809	2.683	2.645	2.554
0.938	0.919	0.904	0.909	2.597	2.511	2.429
1.000	1.000	1.000	1.000	2.499	2.341	2.309
	%AAD	1.124	3.564	%AAD	1.324	1.549

$$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$$

Table 4.23: Vapor-liquid equilibrium pressures and phase compositions for R-23(1)/R-13(2) mixtures with different g^E models (contd.).

x_1	y_1		P (MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		NRTL	UNIQUAC
			UNIQUAC-R			UNIQUAC-R
249.66 K						
0.000	0.000	0.000	0.000	1.218	1.018	1.018
0.043	0.086	0.137	0.133	1.306	1.177	1.168
0.092	0.167	0.233	0.231	1.386	1.313	1.303
0.146	0.237	0.301	0.302	1.458	1.420	1.413
0.200	0.296	0.352	0.356	1.518	1.502	1.500
0.253	0.347	0.392	0.398	1.566	1.563	1.565
0.336	0.429	0.445	0.452	1.623	1.635	1.642
0.397	0.475	0.481	0.487	1.654	1.674	1.683
0.463	0.514	0.518	0.523	1.677	1.704	1.715
0.516	0.549	0.547	0.551	1.692	1.718	1.730
0.594	0.605	0.587	0.590	1.701	1.724	1.738
0.663	0.655	0.622	0.623	1.703	1.714	1.729
0.739	0.712	0.657	0.657	1.691	1.688	1.704
0.800	0.764	0.685	0.684	1.672	1.655	1.671
0.859	0.821	0.716	0.713	1.639	1.607	1.624
0.903	0.867	0.750	0.746	1.606	1.546	1.564
0.938	0.909	0.793	0.786	1.574	1.467	1.486
1.000	1.000	0.999	0.999	1.499	1.148	1.148
	%AAD	12.699	12.817	%AAD	4.420	4.532
						4.554

%AAD = average absolute deviation – defined as $\left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$

Table 4.23: Vapor-liquid equilibrium pressures and phase compositions for R-23(1)/R-13(2) mixtures with different g^E models (contd.).

x ₁	y ₁		P(MPa)				
	exptl	calc		exptl	calc		
		NRTL	UNIQUAC		UNIQUAC-R	NRTL	UNIQUAC
224.61 K							
0.000	0.000	0.000	0.000	0.446	0.427	0.441	0.435
0.043	0.110	0.109	0.109	0.488	0.471	0.480	0.473
0.091	0.196	0.203	0.203	0.520	0.510	0.516	0.509
0.132	0.253	0.266	0.266	0.543	0.536	0.542	0.534
0.198	0.323	0.343	0.343	0.570	0.568	0.573	0.566
0.262	0.377	0.399	0.399	0.589	0.590	0.595	0.587
0.337	0.431	0.449	0.449	0.605	0.607	0.612	0.604
0.433	0.495	0.495	0.495	0.617	0.621	0.623	0.614
0.470	0.516	0.510	0.510	0.620	0.624	0.625	0.617
0.499	0.533	0.521	0.521	0.622	0.625	0.626	0.617
0.665	0.629	0.590	0.590	0.620	0.622	0.620	0.612
0.707	0.656	0.613	0.613	0.617	0.617	0.615	0.606
0.761	0.693	0.650	0.650	0.610	0.608	0.604	0.596
0.825	0.750	0.707	0.707	0.597	0.592	0.585	0.577
0.870	0.798	0.760	0.760	0.583	0.575	0.565	0.557
0.921	0.859	0.835	0.835	0.562	0.548	0.537	0.530
0.953	0.907	0.894	0.894	0.546	0.525	0.516	0.509
1.000	1.000	1.000	1.000	0.513	0.480	0.480	0.474
	%AAD	3.707	3.481	%AAD	1.603	1.737	1.738

%AAD = average absolute deviation – defined as $(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100) / N$

Table 4.23: Vapor-liquid equilibrium pressures and phase compositions for R-23(1)/R-13(2) mixtures with different g^E models.

x ₁	y ₁			P(MPa)		
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		NRTL	UNIQUAC
199.64 K						
0.000	0.000	0.000	0.000	0.154	0.156	0.154
0.049	0.142	0.127	0.138	0.174	0.174	0.172
0.087	0.207	0.200	0.209	0.184	0.184	0.182
0.147	0.291	0.284	0.287	0.195	0.195	0.193
0.213	0.343	0.350	0.348	0.204	0.203	0.201
0.251	0.376	0.381	0.376	0.208	0.207	0.204
0.287	0.396	0.407	0.400	0.210	0.209	0.207
0.412	0.482	0.478	0.468	0.214	0.215	0.212
0.538	0.535	0.539	0.528	0.216	0.216	0.213
0.565	0.548	0.552	0.542	0.216	0.216	0.213
0.564	0.550	0.552	0.541	0.216	0.216	0.213
0.635	0.580	0.588	0.579	0.214	0.215	0.212
0.657	0.591	0.601	0.592	0.214	0.214	0.211
0.668	0.599	0.607	0.598	0.213	0.213	0.210
0.754	0.646	0.663	0.659	0.210	0.209	0.206
0.784	0.673	0.687	0.685	0.208	0.206	0.203
0.815	0.691	0.714	0.714	0.206	0.203	0.200
0.854	0.739	0.754	0.757	0.200	0.199	0.196
0.912	0.812	0.828	0.835	0.190	0.190	0.187
0.975	0.925	0.941	0.946	0.173	0.178	0.176
1.000	1.000	1.000	1.000	0.164	0.172	0.170
	%AAD	2.040	1.368	%AAD	1.046	1.738

%AAD = average absolute deviation – defined as $(\sum abs((exp - calc) / exp) * 100) / N$

R-123(1)/R-13(2)

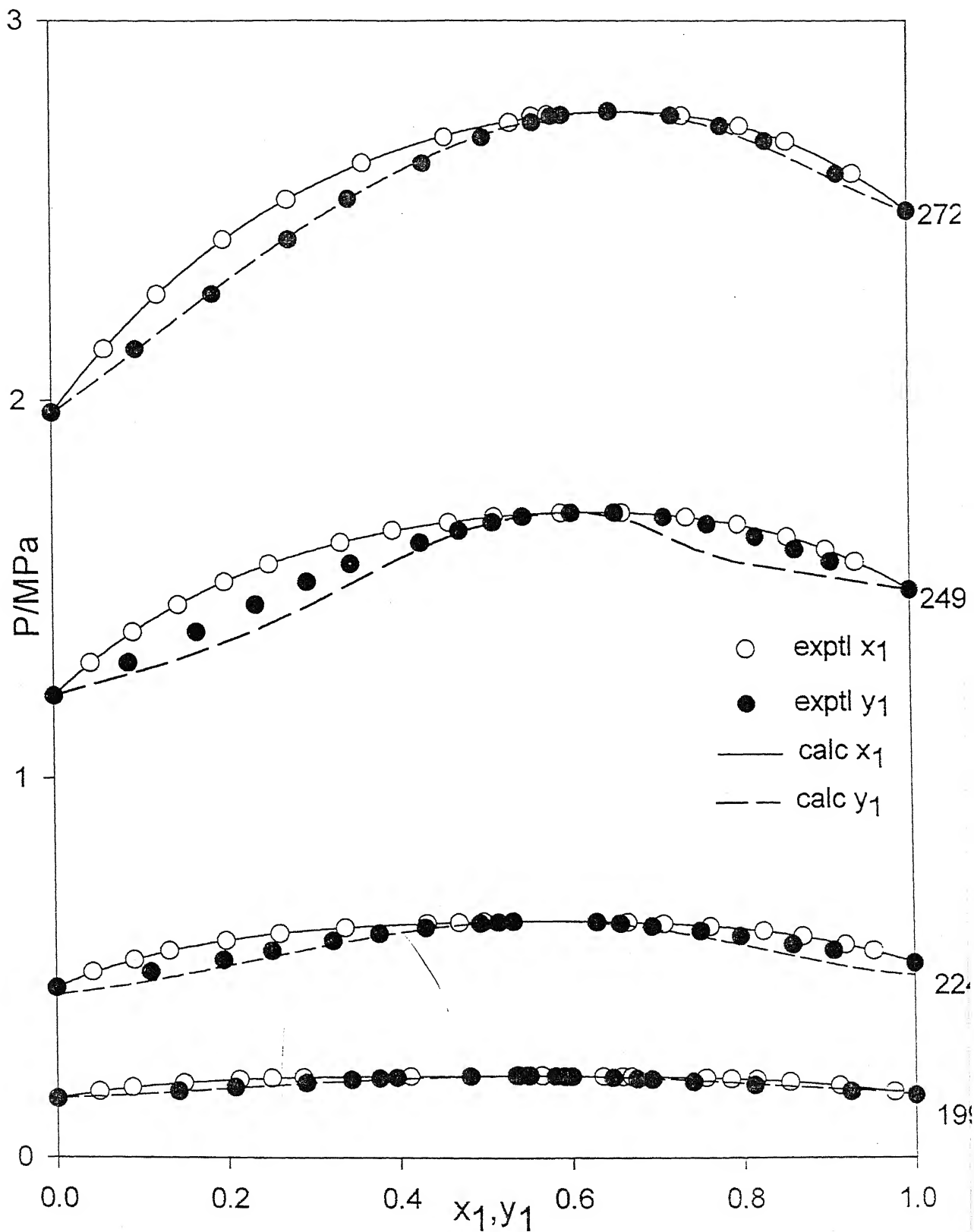


Fig.4.15 Vapor-liquid equilibrium pressures and phase compositions for R-23(1)/R-13(2) mixtures at different temperatures (K).

Table 4.24: Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-123(2) mixtures with different g^E models (contd.).

x ₁	y ₁				P (MPa)			
	exptl	calc		exptl	calc			
		NRTL	UNIQUAC		UNIQUAC-R	NRTL	UNIQUAC	UNIQUAC-R
289.17 K								
0.000	0.000	0.000	0.000	0.073	0.072	0.072	0.072	
0.103	0.495	0.420	0.393	0.120	0.132	0.125	0.125	
0.153	0.593	0.528	0.510	0.145	0.155	0.147	0.146	
0.244	0.720	0.659	0.661	0.195	0.195	0.189	0.188	
0.361	0.802	0.763	0.777	0.249	0.245	0.244	0.245	
0.510	0.860	0.847	0.863	0.312	0.306	0.312	0.311	
0.740	0.926	0.931	0.936	0.393	0.396	0.403	0.401	
1.000	1.000	1.000	1.000	0.521	0.520	0.527	0.524	
	%AAD	6.894	7.842	%AAD	2.840	2.113	1.719	
303.15 K								
0.000	0.000	0.000	0.000	0.121	0.120	0.120	0.121	
0.108	0.481	0.416	0.420	0.201	0.206	0.208	0.208	
0.191	0.629	0.580	0.580	0.264	0.264	0.265	0.265	
0.317	0.736	0.725	0.725	0.356	0.351	0.350	0.351	
0.487	0.822	0.835	0.836	0.464	0.463	0.463	0.463	
0.636	0.880	0.894	0.896	0.553	0.553	0.554	0.554	
0.709	0.897	0.917	0.919	0.594	0.596	0.596	0.595	
0.766	0.915	0.934	0.935	0.628	0.628	0.628	0.628	
1.000	1.000	1.000	1.000	0.768	0.767	0.765	0.766	
	%AAD	4.332	4.301	%AAD	0.634	0.850	0.656	

%AAD = average absolute deviation defined as $(\sum abs((exp - calc)/exp) * 100) / N$

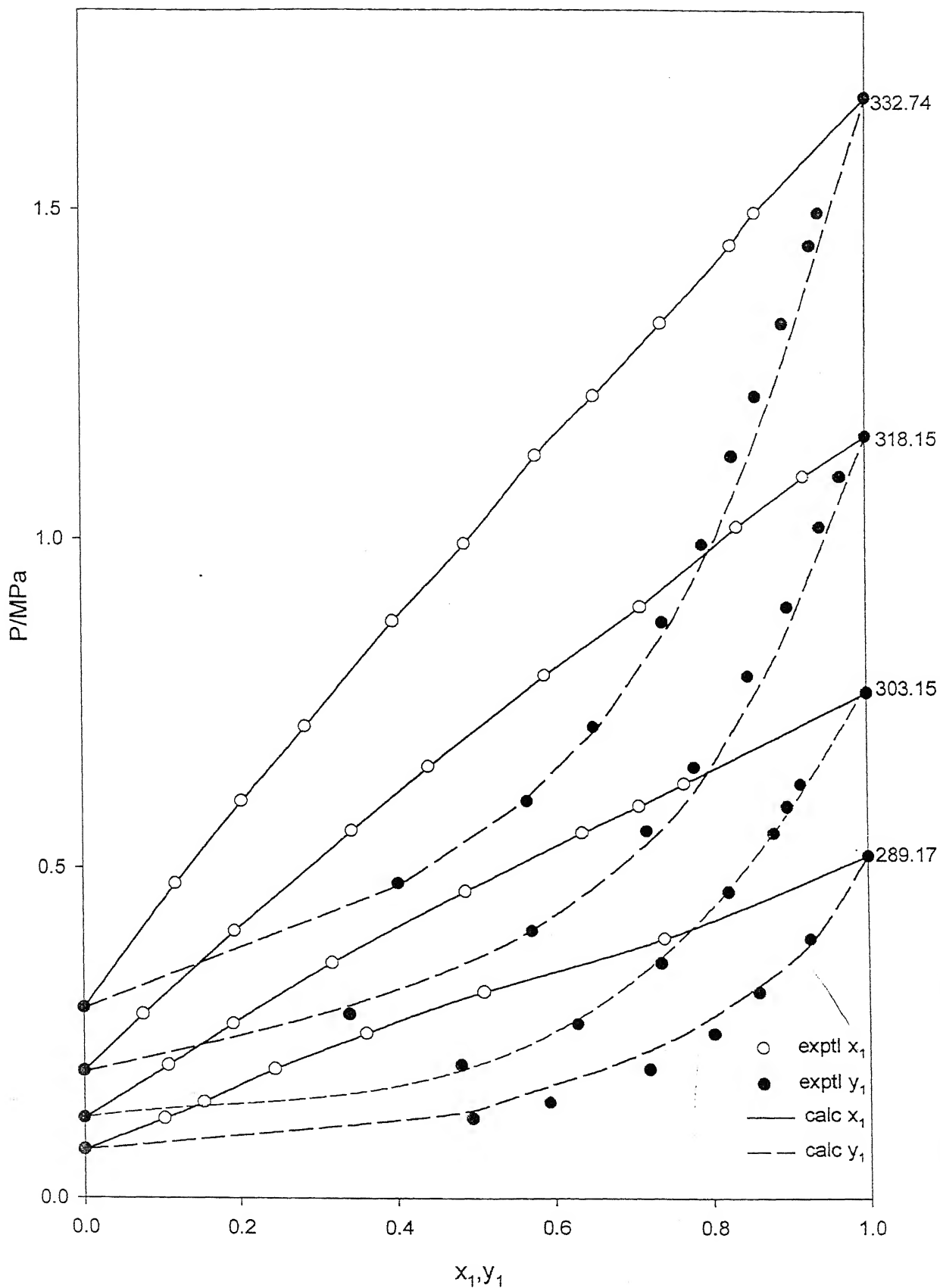


Fig.4.16 Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-123(2) mixtures at different temperatures (K).

Table 4.25: Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-114(2) mixtures with different g^E models (contd.).

x ₁	y ₁				P(MPa)		
	exptl	calc			exptl	calc	
		NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC
253.15 K							
0.000	0.000	0.000	0.000	0.000	0.040	0.040	0.040
0.104	0.522	0.485	0.512	0.512	0.076	0.076	0.076
0.262	0.731	0.739	0.717	0.717	0.116	0.116	0.113
0.583	0.883	0.895	0.889	0.889	0.178	0.187	0.182
0.761	0.932	0.933	0.934	0.934	0.208	0.212	0.209
0.885	0.965	0.962	0.964	0.964	0.229	0.228	0.227
1.000	1.000	1.000	1.000	1.000	0.245	0.256	0.240
	%AAD	1.980	0.945	0.796	%AAD	2.982	1.229
283.15 K							
0.000	0.000	0.000	0.000	0.000	0.131	0.131	0.131
0.065	0.277	0.317	0.370	0.370	0.181	0.182	0.201
0.163	0.542	0.552	0.554	0.555	0.264	0.255	0.263
0.281	0.678	0.696	0.684	0.684	0.336	0.336	0.335
0.423	0.778	0.794	0.789	0.789	0.423	0.422	0.417
0.524	0.825	0.840	0.840	0.841	0.469	0.475	0.475
0.571	0.849	0.858	0.859	0.859	0.498	0.498	0.497
0.747	0.904	0.914	0.916	0.916	0.562	0.574	0.572
0.869	0.945	0.951	0.952	0.952	0.619	0.624	0.623
1.000	1.000	1.000	1.000	1.000	0.681	0.682	0.679
	%AAD	3.175	5.388	4.825	%AAD	1.058	2.039
							1.743

$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$

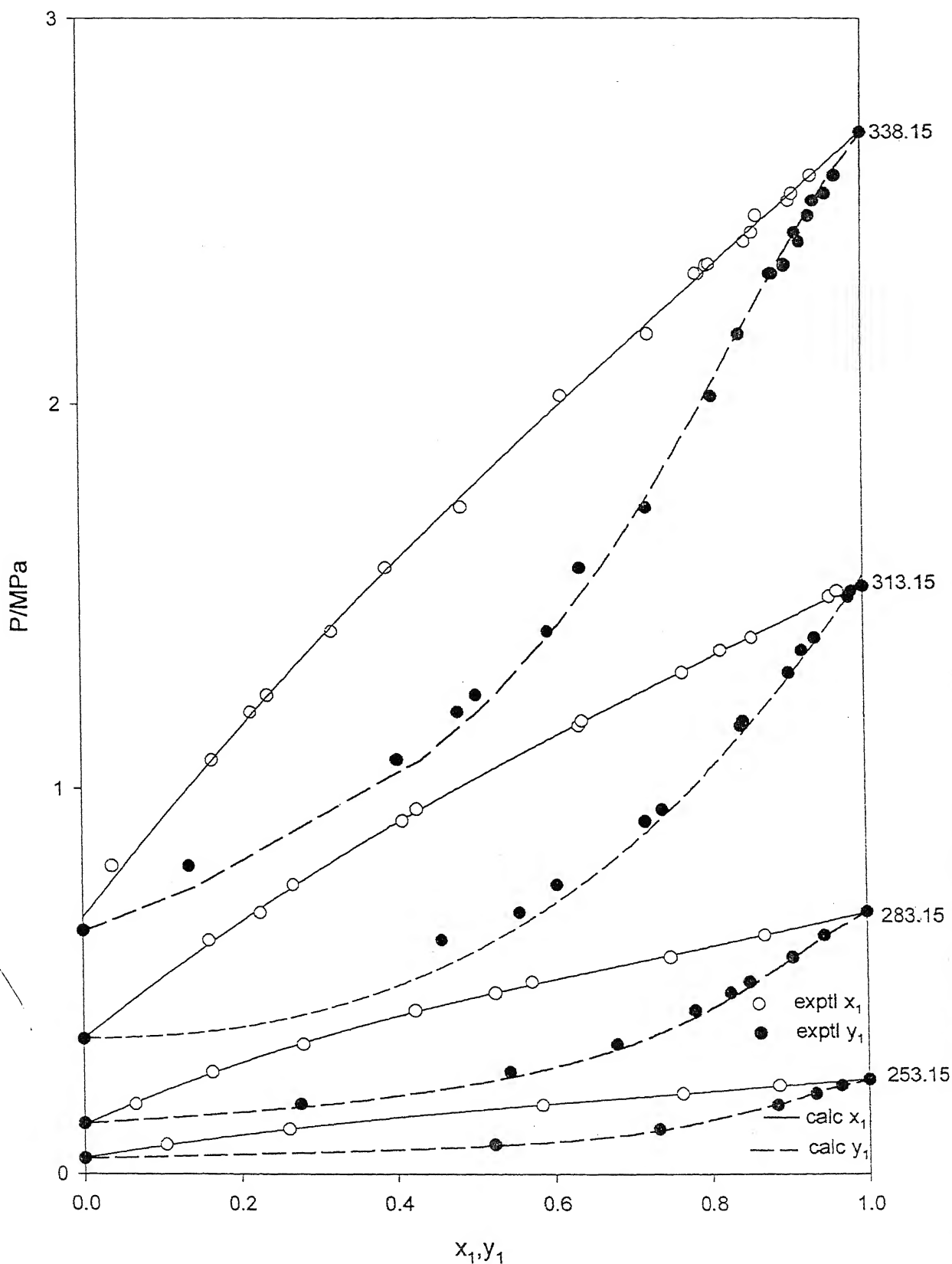


Fig.4.17 Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-114(2) mixtures at different temperatures (K).

Table 4.25: Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-114(2) mixtures with different g^E models.

x_1	y_1		P(MPa)			
	exptl	NRTL	calc		exptl	NRTL
			UNIQUAC	UNIQUAC-R		
338.15 K						
0.000	0.000	0.000	0.000	0.000	0.631	0.630
0.037	0.135	0.144	0.186	0.186	0.799	0.746
0.165	0.403	0.432	0.432	0.431	1.074	1.073
0.216	0.480	0.502	0.496	0.495	1.198	1.194
0.238	0.503	0.527	0.522	0.521	1.242	1.244
0.321	0.595	0.608	0.608	0.607	1.408	1.427
0.391	0.637	0.663	0.671	0.670	1.574	1.574
0.487	0.722	0.725	0.743	0.742	1.732	1.766
0.615	0.808	0.795	0.818	0.817	2.021	2.010
0.726	0.844	0.852	0.870	0.869	2.182	2.216
0.793	0.884	0.885	0.899	0.898	2.339	2.339
0.787	0.887	0.882	0.897	0.896	2.339	2.328
0.802	0.902	0.890	0.903	0.902	2.360	2.355
0.806	0.903	0.892	0.905	0.904	2.363	2.363
0.852	0.922	0.916	0.925	0.924	2.422	2.447
0.862	0.916	0.921	0.929	0.929	2.446	2.465
0.867	0.934	0.924	0.932	0.931	2.490	2.474
0.908	0.940	0.946	0.951	0.951	2.529	2.549
0.913	0.955	0.949	0.953	0.953	2.547	2.558
0.937	0.967	0.962	0.965	0.965	2.594	2.602
1.000	1.000	1.000	1.000	1.000	2.707	2.705
	%AAD	2.082	3.856	3.760	%AAD	0.911
						0.575
						0.631
						0.797
						1.096
						1.198
						1.242
						1.411
						1.558
						1.760
						2.017
						2.222
						2.340
						2.329
						2.355
						2.362
						2.443
						2.460
						2.469
						2.542
						2.551
						2.595
						2.705
						0.586

$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$

Table 4.26: Vapor-liquid equilibrium pressures and phase compositions for R-12(1)/R-114(2) mixtures with different g^E models.

x_1	y_1		P(MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		NRTL	UNIQUAC
						UNIQUAC-R
283.15 K						
0.000	0.000	0.000	0.000	0.130	0.129	0.131
0.426	0.676	0.692	0.679	0.253	0.256	0.258
0.525	0.752	0.766	0.754	0.281	0.284	0.285
0.577	0.791	0.800	0.790	0.299	0.299	0.299
0.665	0.844	0.851	0.843	0.327	0.324	0.323
0.776	0.906	0.906	0.903	0.357	0.355	0.354
0.789	0.912	0.912	0.909	0.363	0.359	0.358
0.859	0.944	0.943	0.942	0.386	0.378	0.378
0.882	0.958	0.953	0.952	0.394	0.385	0.384
1.000	1.000	1.000	1.000	0.417	0.416	0.416
	%AAD	0.869	0.331	%AAD	1.158	1.432
						1.434
313.15 K						
0.000	0.000	0.000	0.000	0.350	0.351	0.351
0.061	0.152	0.154	0.164	0.387	0.376	0.382
0.076	0.178	0.187	0.197	0.399	0.386	0.393
0.228	0.431	0.441	0.439	0.493	0.487	0.491
0.307	0.526	0.535	0.530	0.536	0.537	0.539
0.436	0.654	0.657	0.652	0.616	0.616	0.614
0.523	0.727	0.725	0.721	0.668	0.668	0.664
0.616	0.793	0.788	0.786	0.719	0.722	0.717
0.752	0.878	0.868	0.869	0.810	0.798	0.795
0.814	0.913	0.902	0.904	0.846	0.833	0.830
0.882	0.947	0.938	0.940	0.896	0.871	0.869
1.000	1.000	1.000	1.000	0.936	0.935	0.935
	%AAD	1.541	2.629	%AAD	1.359	1.166
						1.045

$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \frac{\text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100}{N} \right) / N$

R-12(1)/R-114(2)

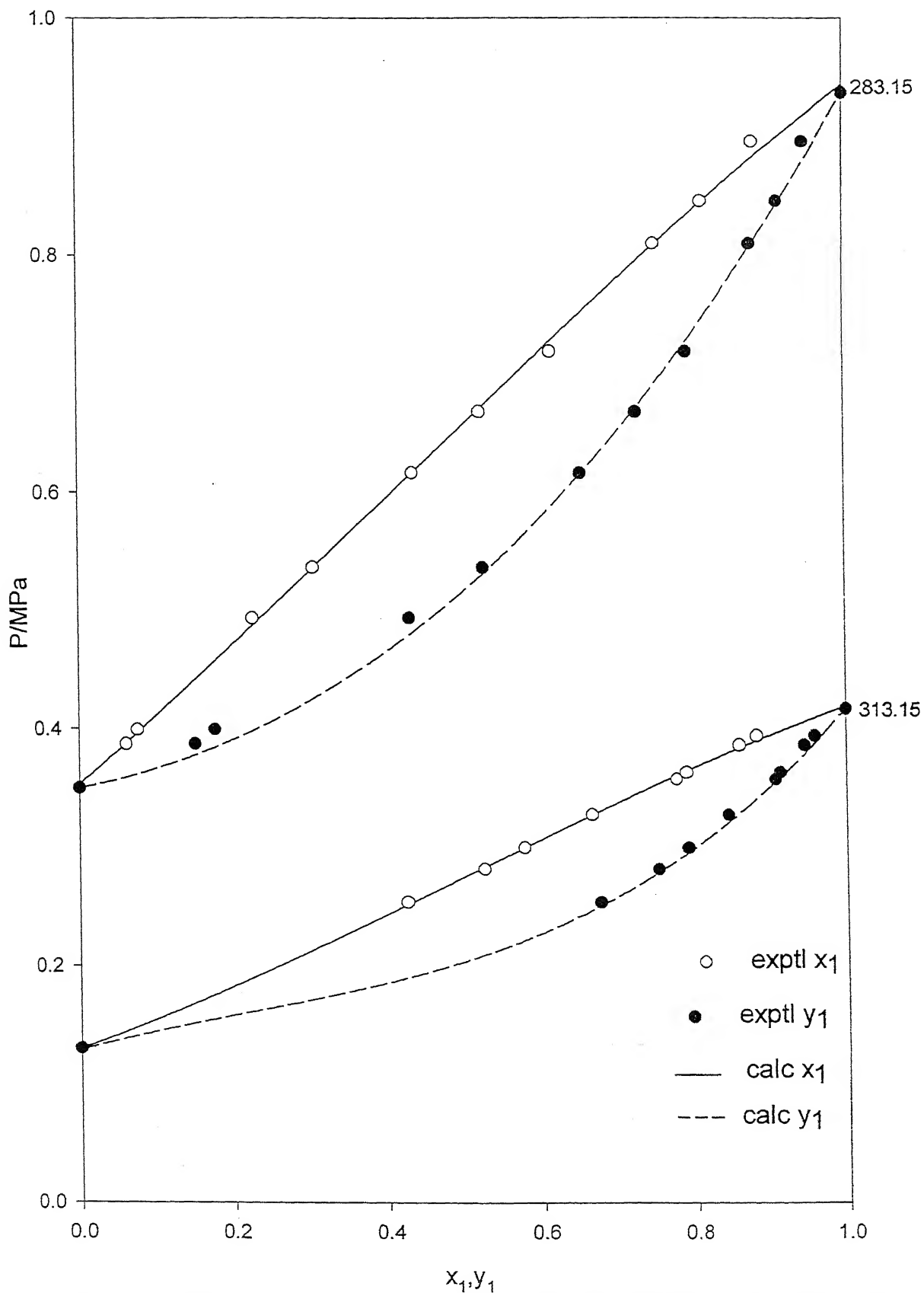


Fig.4.18 Vapor-liquid equilibrium pressures and phase compositions for R-12(1)/R-114(2) mixtures at different temperatures (K).

Table 4.27: Vapor-liquid equilibrium pressures and phase compositions for R13B1(1)/R-12(2) mixtures with different g^E models (contd.).

x ₁	y ₁				P(MPa)			
	exptl	calc		exptl	calc			
		NRTL	UNIQUAC		UNIQUAC-R	NRTL	UNIQUAC	UNIQUAC-R
253.15 K								
0.000	0.000	0.000	0.000	0.000	0.142	0.140	0.141	0.142
0.204	0.420	0.394	0.389	0.389	0.207	0.207	0.207	0.207
0.403	0.657	0.640	0.638	0.638	0.264	0.263	0.262	0.262
0.564	0.791	0.777	0.778	0.778	0.311	0.311	0.311	0.311
0.746	0.893	0.889	0.891	0.891	0.365	0.368	0.368	0.368
0.887	0.959	0.956	0.956	0.956	0.411	0.413	0.413	0.413
1.000	1.000	0.999	1.000	1.000	0.442	0.442	0.441	0.442
	%AAD	2.257	2.511	2.507	%AAD	0.305	0.424	0.423

$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$

Table 4.27: Vapor-liquid equilibrium pressures and phase compositions for R13B1(1)/R-12(2) mixtures with different g^E models (contd.).

x_1	y_1			P(MPa)			
	exptl	calc		exptl	calc		
		NRTL	UNIQUAC		UNIQUAC	NRTL	UNIQUAC-R
283.15 K							
0.000	0.000	0.000	0.000	0.420	0.421	0.421	0.421
0.061	0.117	0.135	0.147	0.463	0.458	0.470	0.470
0.084	0.167	0.181	0.188	0.477	0.474	0.485	0.485
0.144	0.271	0.290	0.284	0.523	0.516	0.522	0.522
0.261	0.414	0.464	0.451	0.597	0.599	0.598	0.598
0.262	0.453	0.465	0.452	0.600	0.600	0.599	0.599
0.283	0.472	0.492	0.479	0.618	0.615	0.613	0.613
0.345	0.539	0.562	0.553	0.658	0.659	0.656	0.656
0.447	0.627	0.659	0.656	0.721	0.730	0.728	0.728
0.449	0.640	0.661	0.658	0.729	0.732	0.729	0.729
0.523	0.700	0.720	0.720	0.776	0.782	0.781	0.781
0.605	0.760	0.777	0.778	0.836	0.836	0.836	0.836
0.682	0.820	0.825	0.827	0.887	0.886	0.886	0.886
0.729	0.840	0.852	0.854	0.915	0.915	0.916	0.916
0.750	0.856	0.864	0.866	0.934	0.928	0.929	0.929
0.828	0.900	0.907	0.908	0.983	0.977	0.977	0.977
0.833	0.908	0.910	0.911	0.992	0.980	0.981	0.981
0.872	0.934	0.931	0.931	1.017	1.004	1.005	1.005
0.935	0.965	0.965	0.965	1.066	1.044	1.044	1.044
1.000	1.000	1.000	1.000	1.101	1.100	1.101	1.101
	%AAD	3.987	4.108	%AAD	0.703	0.672	0.673

%AAD = average absolute deviation -- defined as $(\sum abs((exp - calc) / exp) * 100) / N$

Table 4.27: Vapor-liquid equilibrium pressures and phase compositions for R13B1(1)/R-12(2) mixtures with different g^E models.

x ₁	y ₁				P(MPa)			
	exptl	calc			exptl	calc		
		NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
313.15 K								
0.000	0.000	0.000	0.000	0.000	0.980	0.990	0.979	0.981
0.088	0.158	0.167	0.173	0.173	1.069	1.054	1.069	1.069
0.093	0.166	0.176	0.181	0.181	1.076	1.060	1.075	1.076
0.186	0.305	0.319	0.316	0.316	1.184	1.184	1.194	1.194
0.251	0.394	0.404	0.399	0.400	1.274	1.271	1.276	1.276
0.340	0.499	0.505	0.501	0.501	1.391	1.389	1.390	1.390
0.392	0.550	0.558	0.555	0.555	1.457	1.457	1.457	1.457
0.486	0.618	0.642	0.643	0.642	1.573	1.580	1.579	1.579
0.519	0.668	0.670	0.671	0.670	1.622	1.623	1.622	1.622
0.609	0.741	0.739	0.741	0.741	1.732	1.739	1.739	1.739
0.706	0.812	0.807	0.810	0.810	1.869	1.864	1.864	1.864
0.797	0.874	0.868	0.870	0.870	1.991	1.981	1.981	1.982
0.867	0.919	0.913	0.914	0.914	2.087	2.073	2.073	2.073
1.000	1.000	1.000	1.000	1.000	2.251	2.244	2.251	2.252
	%AAD	2.335	2.521	2.535	%AAD	0.476	0.284	0.283

$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$

Table 4.28: Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-142b(2) mixtures with different g^E models (contd.).

x_1	y_1		$P(\text{MPa})$				
	exptl	calc		exptl	calc		
		NRTL	UNIQUAC		UNIQUAC-R	NRTL	UNIQUAC
273.15 K							
0.000	0.000	0.000	0.000	0.000	0.146	0.145	0.145
0.127	0.291	0.301	0.316	0.316	0.184	0.182	0.191
0.203	0.438	0.436	0.432	0.432	0.211	0.207	0.213
0.288	0.574	0.557	0.543	0.543	0.239	0.236	0.240
0.356	0.645	0.635	0.620	0.620	0.263	0.260	0.262
0.484	0.756	0.751	0.741	0.741	0.308	0.306	0.307
0.522	0.780	0.779	0.770	0.770	0.320	0.320	0.319
0.579	0.817	0.817	0.811	0.811	0.341	0.341	0.341
0.627	0.836	0.846	0.841	0.841	0.358	0.359	0.358
0.714	0.891	0.890	0.888	0.888	0.390	0.391	0.390
0.772	0.915	0.917	0.915	0.915	0.411	0.412	0.412
0.794	0.924	0.926	0.925	0.925	0.417	0.420	0.417
0.815	0.936	0.934	0.934	0.934	0.427	0.428	0.428
0.838	0.945	0.943	0.943	0.943	0.436	0.437	0.437
0.857	0.951	0.951	0.950	0.950	0.442	0.444	0.444
1.000	1.000	1.000	1.000	1.000	0.498	0.497	0.497
	%AAD	0.698	1.550	1.653	%AAD	0.593	0.597
							0.473

%AAD = average absolute deviation – defined as $(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100) / N$

Table 4.28: Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-142b(2) mixtures with different g^E models (contd.).

x ₁	y ₁				P(MPa)			
	exptl	calc			exptl	calc		
		NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
263.15 K								
0.000	0.000	0.000	0.000	0.000	0.098	0.098	0.098	0.098
0.068	0.155	0.185	0.200	0.200	0.112	0.112	0.115	0.114
0.101	0.246	0.262	0.271	0.271	0.121	0.120	0.122	0.121
0.265	0.539	0.544	0.536	0.537	0.161	0.159	0.160	0.161
0.394	0.646	0.689	0.683	0.683	0.193	0.192	0.192	0.193
0.448	0.713	0.736	0.732	0.732	0.208	0.207	0.206	0.206
0.525	0.771	0.793	0.791	0.791	0.227	0.227	0.227	0.227
0.543	0.785	0.805	0.804	0.804	0.232	0.232	0.232	0.231
0.573	0.802	0.824	0.823	0.823	0.240	0.240	0.240	0.241
0.631	0.846	0.857	0.857	0.857	0.255	0.256	0.256	0.255
0.666	0.869	0.875	0.875	0.875	0.264	0.265	0.265	0.254
0.712	0.893	0.896	0.897	0.897	0.276	0.277	0.278	0.277
0.790	0.932	0.929	0.929	0.929	0.298	0.298	0.298	0.298
0.934	0.983	0.980	0.980	0.980	0.336	0.336	0.337	0.336
1.000	1.000	1.000	1.000	1.000	0.355	0.354	0.354	0.354
	%AAD	3.208	3.938	4.203	%AAD	0.342	0.558	0.563

%AAD = average absolute deviation defined as $(\sum abs((exp - calc) / exp) * 100) / N$

Table 4.28: Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-142b(2) mixtures with different g^E models (contd.).

x ₁	y ₁		P (MPa)				
	exptl	NRTL	calc		exptl	calc	
			UNIQUAC	UNIQUAC-R		UNIQUAC	UNIQUAC-R
283.15 K							
0.000	0.000	0.000	0.000	0.000	0.210	0.207	0.207
0.142	0.312	0.331	0.334	0.334	0.271	0.271	0.278
0.304	0.543	0.562	0.550	0.550	0.345	0.345	0.345
0.463	0.707	0.714	0.709	0.709	0.418	0.418	0.416
0.527	0.750	0.762	0.760	0.760	0.447	0.448	0.447
0.571	0.783	0.793	0.792	0.792	0.471	0.469	0.468
0.597	0.800	0.809	0.810	0.810	0.481	0.481	0.481
0.665	0.842	0.850	0.852	0.852	0.514	0.514	0.514
0.693	0.856	0.866	0.867	0.867	0.524	0.527	0.528
0.725	0.872	0.882	0.884	0.884	0.541	0.543	0.543
0.748	0.886	0.894	0.896	0.896	0.554	0.554	0.555
0.780	0.900	0.910	0.911	0.911	0.565	0.570	0.571
0.792	0.911	0.915	0.917	0.917	0.575	0.576	0.576
0.863	0.946	0.947	0.948	0.948	0.607	0.611	0.612
0.889	0.954	0.958	0.958	0.958	0.627	0.624	0.625
1.000	1.000	1.000	1.000	1.000	0.679	0.680	0.680
	%AAD	1.298	1.255	1.243	%AAD	0.337	0.558
							0.556
							0.576
							0.612
							0.625
							0.680
							0.558

$$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$$

Table 4.28: Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-142b(2) mixtures with different g^E models (contd.).

x ₁	y ₁		P (MPa)				
	exptl	NRTL	calc		exptl	calc	
			UNIQUAC	UNIQUAC-R		UNIQUAC	UNIQUAC-R
293.15 K							
0.000	0.000	0.000	0.000	0.000	0.293	0.289	0.289
0.118	0.259	0.274	0.276	0.276	0.360	0.359	0.366
0.173	0.351	0.370	0.361	0.361	0.393	0.391	0.394
0.244	0.455	0.473	0.460	0.459	0.432	0.433	0.432
0.311	0.542	0.554	0.543	0.543	0.474	0.473	0.469
0.436	0.670	0.678	0.674	0.674	0.545	0.549	0.544
0.518	0.733	0.743	0.745	0.745	0.595	0.599	0.595
0.570	0.783	0.780	0.784	0.784	0.629	0.631	0.629
0.609	0.805	0.806	0.811	0.811	0.657	0.655	0.654
0.636	0.821	0.823	0.828	0.828	0.672	0.672	0.672
0.657	0.831	0.836	0.841	0.841	0.688	0.685	0.685
0.696	0.854	0.859	0.863	0.863	0.710	0.710	0.711
0.737	0.880	0.881	0.885	0.885	0.735	0.736	0.737
0.782	0.902	0.904	0.908	0.908	0.764	0.765	0.767
0.811	0.921	0.918	0.921	0.921	0.785	0.784	0.785
0.827	0.925	0.926	0.929	0.929	0.795	0.795	0.796
0.861	0.941	0.942	0.944	0.944	0.814	0.817	0.818
0.873	0.946	0.947	0.949	0.949	0.824	0.825	0.826
0.897	0.959	0.958	0.959	0.959	0.846	0.841	0.841
0.919	0.970	0.967	0.968	0.968	0.857	0.855	0.856
1.000	1.000	1.000	1.000	1.000	0.910	0.910	0.910
	%AAD	1.102	0.931	0.923	%AAD	0.313	0.366
							0.367

$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$

Table 4.28: Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-142b(2) mixtures
with different g^E models (contd.).

x ₁	y ₁				P(MPa)			
	exptl	calc		exptl	calc			
		NRTL	UNIQUAC		UNIQUAC-R	NRTL	UNIQUAC	UNIQUAC-R
313.15 K								
0.000	0.000	0.000	0.000	0.526	0.525	0.526	0.525	
0.072	0.155	0.162	0.166	0.589	0.592	0.589	0.599	
0.079	0.172	0.176	0.179	0.596	0.599	0.596	0.605	
0.095	0.200	0.207	0.206	0.618	0.614	0.618	0.618	
0.211	0.392	0.390	0.379	0.720	0.720	0.720	0.711	
0.269	0.472	0.464	0.455	0.769	0.773	0.769	0.759	
0.321	0.525	0.524	0.519	0.799	0.820	0.799	0.805	
0.406	0.610	0.610	0.613	0.906	0.899	0.906	0.884	
0.469	0.677	0.666	0.676	0.965	0.959	0.965	0.947	
0.563	0.749	0.742	0.756	1.059	1.050	1.059	1.044	
0.574	0.761	0.751	0.765	1.063	1.061	1.063	1.056	
0.631	0.803	0.792	0.806	1.113	1.119	1.113	1.118	
0.653	0.815	0.807	0.821	1.138	1.141	1.138	1.142	
0.736	0.869	0.861	0.873	1.230	1.230	1.230	1.233	
0.800	0.906	0.900	0.908	1.287	1.301	1.287	1.305	
0.804	0.908	0.902	0.910	1.304	1.305	1.304	1.310	
0.837	0.925	0.921	0.926	1.347	1.343	1.347	1.347	
1.000	1.000	1.000	1.000	1.534	1.537	1.534	1.537	
	%AAD	1.210	1.468	%AAD	0.563	0.895	0.893	

%AAD = average absolute deviation – defined as $(\sum abs((exp - calc) / exp) * 100) / N$

Table 4.28: Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-142b(2) mixtures with different g^E models.

x ₁	y ₁		P(MPa)				
	exptl	calc		exptl	calc		
		NRTL	UNIQUAC		UNIQUAC-R	NRTL	UNIQUAC
338.15 K							
0.000	0.000	0.000	0.000	0.000	0.995	0.991	0.991
0.104	0.194	0.190	0.196	0.196	1.133	1.127	1.152
0.153	0.276	0.269	0.268	0.268	1.219	1.197	1.218
0.247	0.398	0.404	0.397	0.396	1.334	1.338	1.348
0.415	0.591	0.597	0.594	0.593	1.626	1.611	1.610
0.497	0.665	0.674	0.674	0.673	1.766	1.753	1.751
0.594	0.744	0.752	0.755	0.754	1.926	1.926	1.925
0.633	0.777	0.780	0.784	0.783	1.999	1.997	1.997
0.664	0.796	0.802	0.805	0.805	2.052	2.054	2.055
0.732	0.845	0.846	0.850	0.850	2.180	2.181	2.182
0.829	0.895	0.905	0.907	0.907	2.328	2.367	2.368
0.880	0.925	0.934	0.935	0.935	2.437	2.467	2.468
1.000	1.000	1.000	1.000	1.000	2.704	2.715	2.715
	%AAD	0.998	0.937	0.917	%AAD	0.628	0.682

%AAD = average absolute deviation -- defined as $(\sum abs((exp - calc) / exp) * 100) / N$

Table 4.29: Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-142b(2) mixtures with different g^E models (contd.).

x ₁	y ₁				P (MPa)			
	exptl	calc			exptl	calc		
		NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
295.45 K								
0.000	0.000	0.000	0.000	0.000	0.307	0.308	0.311	0.311
0.122	0.403	0.412	0.408	0.407	0.484	0.482	0.481	0.480
0.339	0.698	0.702	0.707	0.704	0.780	0.780	0.780	0.777
0.427	0.758	0.765	0.771	0.769	0.892	0.894	0.895	0.891
0.633	0.854	0.867	0.872	0.869	1.143	1.143	1.143	1.138
0.772	0.914	0.918	0.921	0.920	1.306	1.301	1.297	1.294
0.863	0.948	0.950	0.951	0.951	1.414	1.403	1.399	1.397
1.000	1.000	1.000	1.000	1.000	1.582	1.565	1.565	1.565
	%AAD	0.741	0.914	0.742	%AAD	0.388	0.664	0.791
304.55 K								
0.000	0.000	0.000	0.000	0.000	0.404	0.407	0.410	0.410
0.116	0.363	0.378	0.372	0.371	0.610	0.608	0.604	0.604
0.329	0.667	0.678	0.680	0.679	0.968	0.972	0.969	0.967
0.437	0.750	0.760	0.763	0.762	1.149	1.149	1.149	1.146
0.619	0.840	0.853	0.857	0.856	1.412	1.428	1.431	1.427
0.774	0.907	0.913	0.915	0.915	1.663	1.648	1.650	1.648
0.868	0.944	0.947	0.949	0.948	1.806	1.780	1.781	1.780
1.000	1.000	1.000	1.000	1.000	2.016	1.977	1.977	1.977
	%AAD	1.229	1.197	1.103	%AAD	0.859	1.018	1.062

%AAD = average absolute deviation – defined as $(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100) / N$

Table 4.29: Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-142b(2) mixtures with different g^E models.

x ₁	y ₁		P(MPa)					
	exptl	calc		exptl	calc			
		NRTL	UNIQUAC		UNIQUAC-R	NRTL	UNIQUAC	UNIQUAC-R
314.95 K								
0.000	0.000	0.000	0.000	0.000	0.543	0.547	0.551	
0.111	0.340	0.350	0.336	0.333	0.783	0.799	0.781	
0.330	0.631	0.640	0.641	0.634	1.240	1.245	1.229	
0.435	0.725	0.720	0.723	0.717	1.446	1.446	1.443	
0.630	0.828	0.831	0.834	0.830	1.838	1.814	1.843	
0.770	0.898	0.897	0.896	0.895	2.169	2.085	2.131	
0.870	0.938	0.942	0.938	0.938	2.330	2.288	2.330	
1.000	1.000	1.000	1.000	1.000	2.614	2.566	2.566	
	%AAD	0.734	0.495	0.536	%AAD	1.511	1.077	0.845

%AAD = average absolute deviation defined as $(\sum abs((exp - calc) / exp) * 100) / N$

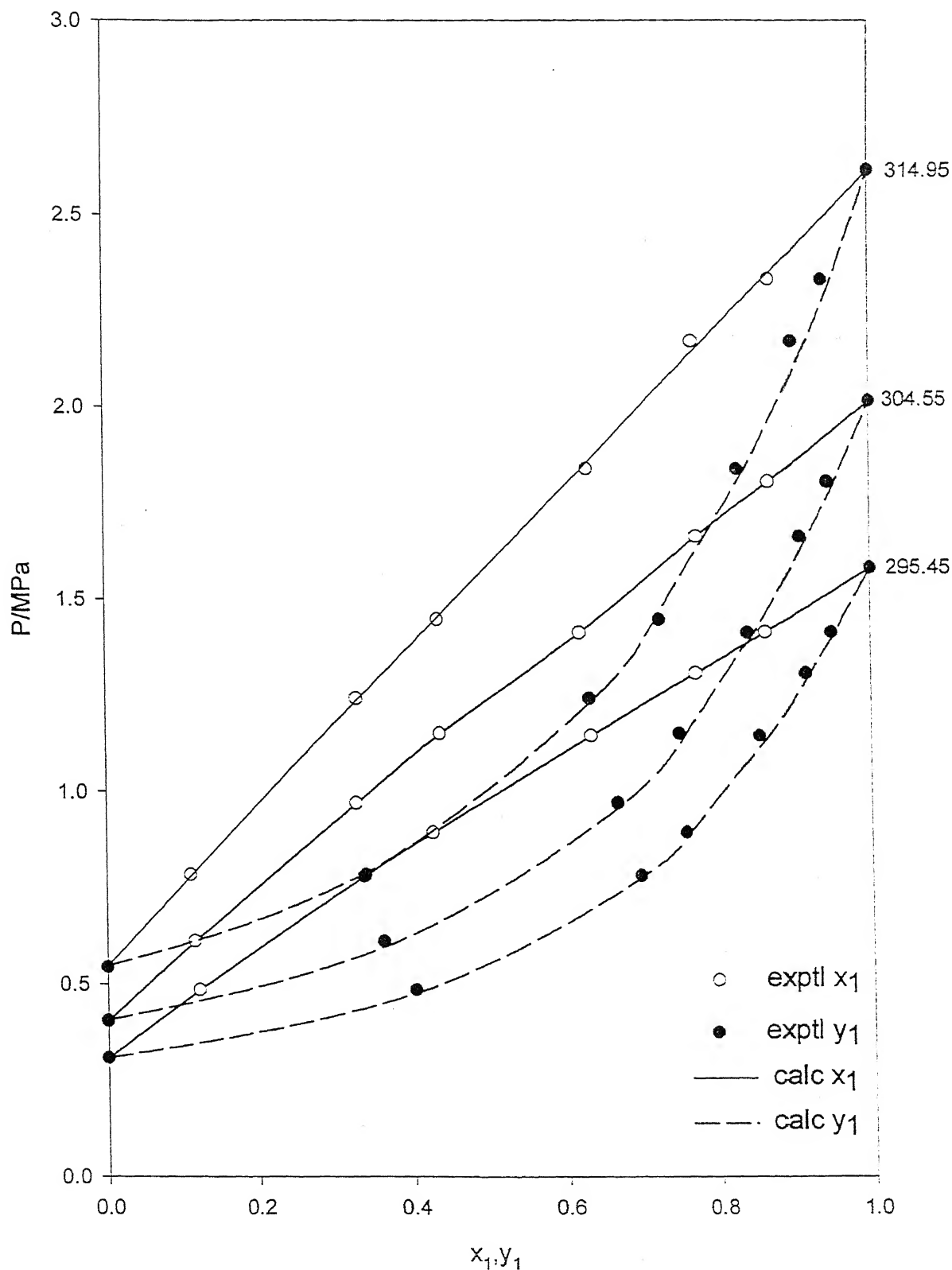


Fig. 4.19 Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-142b(2) mixtures at different temperatures (K).

Table 4.30: Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-123(2) mixtures
with different g^E models (contd.).

x ₁	y ₁		P(MPa)					
	exptl	NRTL	calc		exptl	calc		
			UNIQUAC	UNIQUAC-R			NRTL	UNIQUAC
294.95 K								
0.000	0.000	0.000	0.000	0.000	0.082	0.101	0.101	0.101
0.107	0.730	0.652	0.654	0.654	0.268	0.276	0.278	0.277
0.298	0.895	0.853	0.853	0.853	0.573	0.573	0.573	0.572
0.348	0.899	0.875	0.875	0.875	0.652	0.647	0.646	0.646
0.483	0.927	0.915	0.916	0.915	0.824	0.836	0.835	0.835
0.600	0.950	0.939	0.939	0.933	0.988	0.990	0.990	0.990
0.683	0.962	0.952	0.953	0.952	1.096	1.096	1.096	1.096
0.772	0.973	0.965	0.966	0.965	1.214	1.209	1.209	1.209
1.000	1.000	1.000	1.000	1.000	1.554	1.530	1.530	1.534
	%AAD	2.496	2.416	2.813	%AAD	3.530	3.590	3.475
304.55 K								
0.000	0.000	0.000	0.000	0.000	0.116	0.137	0.137	0.137
0.147	0.751	0.702	0.704	0.704	0.427	0.430	0.432	0.432
0.228	0.828	0.792	0.795	0.794	0.591	0.589	0.590	0.590
0.249	0.842	0.809	0.811	0.811	0.627	0.629	0.630	0.631
0.362	0.891	0.869	0.871	0.871	0.844	0.843	0.843	0.843
0.465	0.917	0.903	0.905	0.905	1.030	1.030	1.030	1.030
0.591	0.942	0.931	0.933	0.934	1.225	1.250	1.249	1.250
1.000	1.000	1.000	1.000	1.000	1.998	1.976	1.976	1.978
	%AAD	2.498	2.296	2.314	%AAD	2.912	2.955	3.021

%AAD = average absolute deviation – defined as $(\sum \text{abs}(\text{exp} - \text{calc}) / \text{exp}) * 100 / N$

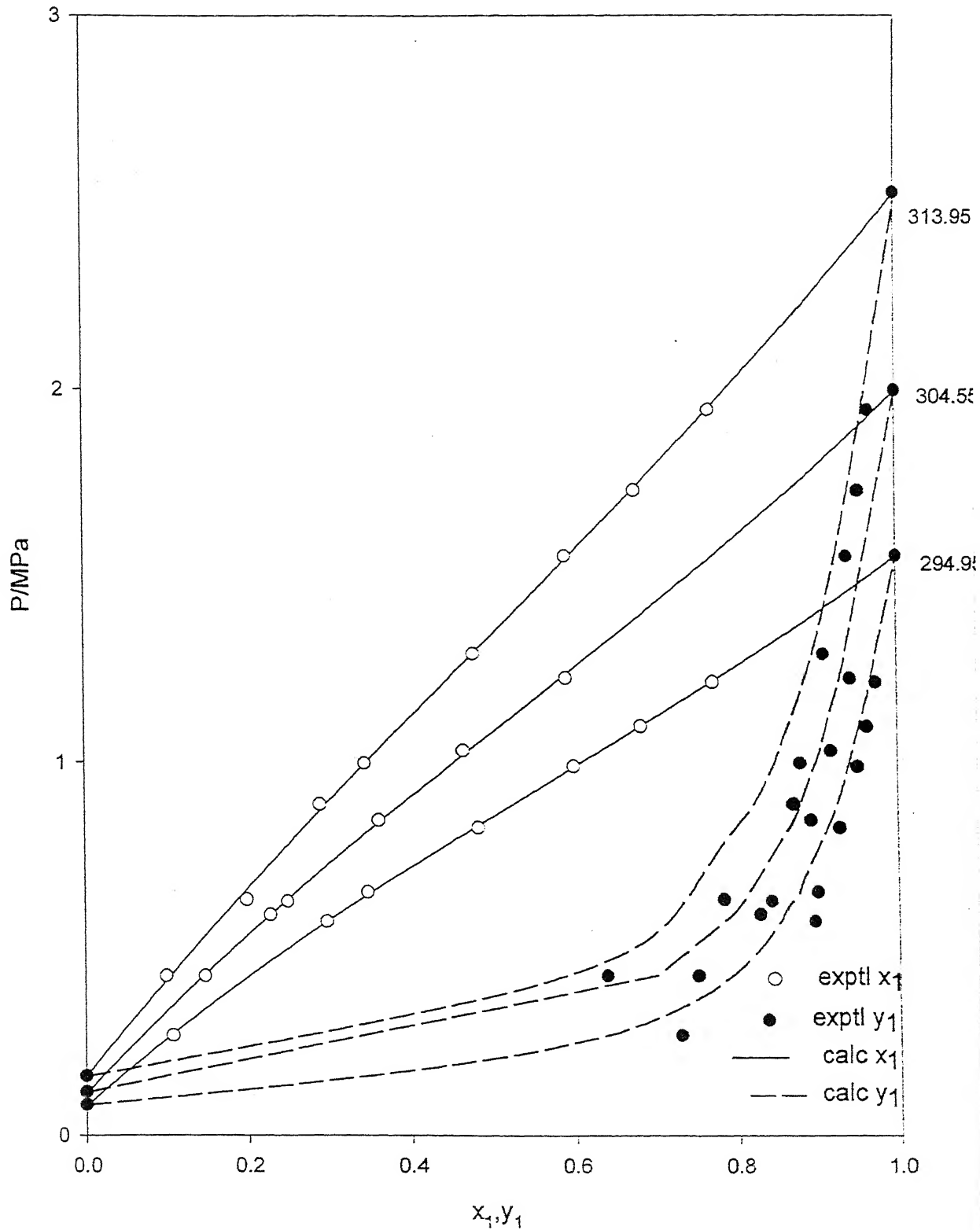


Fig.4.20 Vapor-liquid equilibrium pressures and phase compositions for R-32(1)/R-123(2) mixtures at different temperatures (K).

Table 4.31: Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-600a(2) mixtures with different g^E models (contd.).

x ₁	y ₁				P(MPa)			
	exptl	calc			exptl	calc		
		NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
293.66 K								
0.000	0.000	0.000	0.000	0.000	0.307	0.306	0.306	0.306
0.063	0.282	0.287	0.297	0.297	0.426	0.420	0.423	0.423
0.097	0.381	0.368	0.377	0.377	0.473	0.465	0.468	0.468
0.098	0.375	0.370	0.379	0.379	0.470	0.467	0.469	0.469
0.108	0.385	0.388	0.398	0.398	0.479	0.478	0.481	0.480
0.124	0.417	0.413	0.423	0.423	0.495	0.495	0.497	0.497
0.195	0.493	0.494	0.508	0.509	0.552	0.554	0.556	0.556
0.229	0.518	0.519	0.537	0.537	0.569	0.574	0.578	0.578
0.297	0.561	0.559	0.580	0.580	0.602	0.605	0.610	0.611
0.453	0.624	0.619	0.636	0.636	0.644	0.645	0.648	0.648
0.528	0.648	0.643	0.651	0.651	0.655	0.656	0.655	0.655
0.568	0.661	0.656	0.659	0.659	0.662	0.661	0.658	0.658
0.651	0.690	0.684	0.677	0.678	0.667	0.667	0.661	0.661
0.744	0.730	0.724	0.712	0.712	0.669	0.667	0.660	0.660
0.798	0.758	0.754	0.744	0.744	0.666	0.663	0.655	0.655
0.903	0.843	0.842	0.846	0.846	0.641	0.639	0.628	0.628
1.000	1.000	1.000	1.000	1.000	0.580	0.578	0.578	0.578
	%AAD	0.802	1.829	1.831	%AAD	0.436	0.808	0.810

%AAD = average absolute deviation – defined as $(\sum abs((exp - calc) / exp) * 100) / N$

R-134a(1)/R-600a(2)

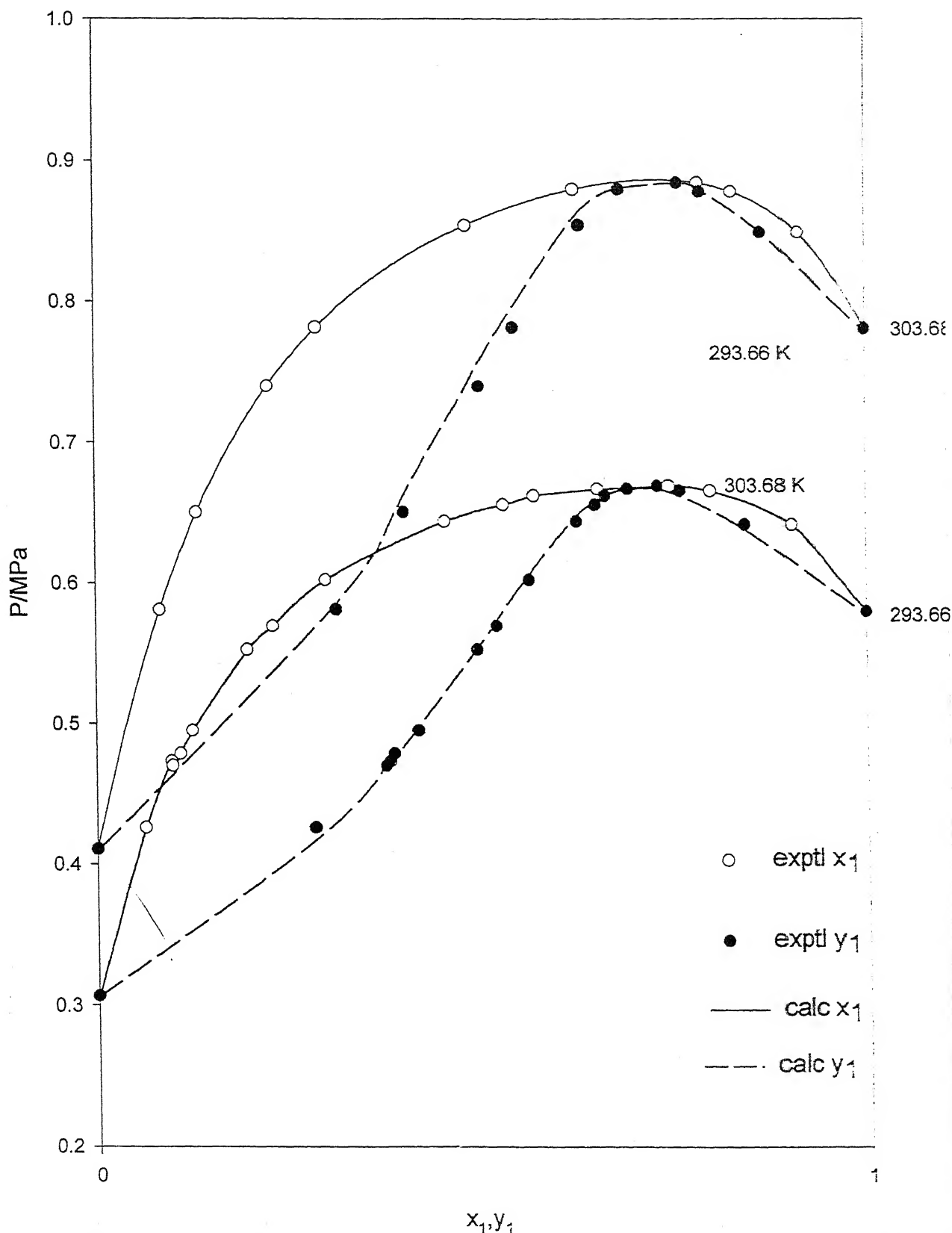


Fig.4.21 Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-600a(2) mixtures at different temperatures (K).

Table 4.32: Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-236fa(2) mixtures with different g^E models.

x_1	y_1		P (MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		NRTL	UNIQUAC
			UNIQUAC-R			UNIQUAC-R
283.62 K						
0.000	0.000	0.000	0.000	0.163	0.168	0.168
0.115	0.236	0.220	0.219	0.191	0.192	0.197
0.257	0.450	0.438	0.418	0.225	0.225	0.225
0.363	0.572	0.568	0.554	0.252	0.251	0.250
0.491	0.694	0.696	0.691	0.284	0.284	0.283
0.606	0.782	0.786	0.786	0.314	0.315	0.314
0.722	0.859	0.862	0.863	0.345	0.345	0.346
0.864	0.937	0.935	0.931	0.384	0.382	0.381
1.000	1.000	0.999	1.000	0.451	0.450	0.458
	%AAD	1.594	2.685	%AAD	0.704	1.192
303.68 K						
0.000	0.000	0.000	0.000	0.326	0.325	0.325
0.110	0.206	0.204	0.215	0.373	0.368	0.387
0.274	0.440	0.447	0.422	0.442	0.438	0.446
0.402	0.585	0.593	0.570	0.499	0.497	0.497
0.509	0.681	0.692	0.677	0.545	0.546	0.544
0.602	0.759	0.767	0.758	0.588	0.590	0.587
0.715	0.839	0.843	0.841	0.641	0.643	0.641
0.794	0.888	0.891	0.891	0.680	0.680	0.676
0.898	0.948	0.949	0.949	0.730	0.729	0.728
1.000	1.000	1.000	1.000	0.781	0.778	0.778
	%AAD	0.690	1.276	%AAD	0.374	0.692

%AAD = average absolute deviation - defined as $(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100) / N$

R-134a(1)/R-236fa(2)

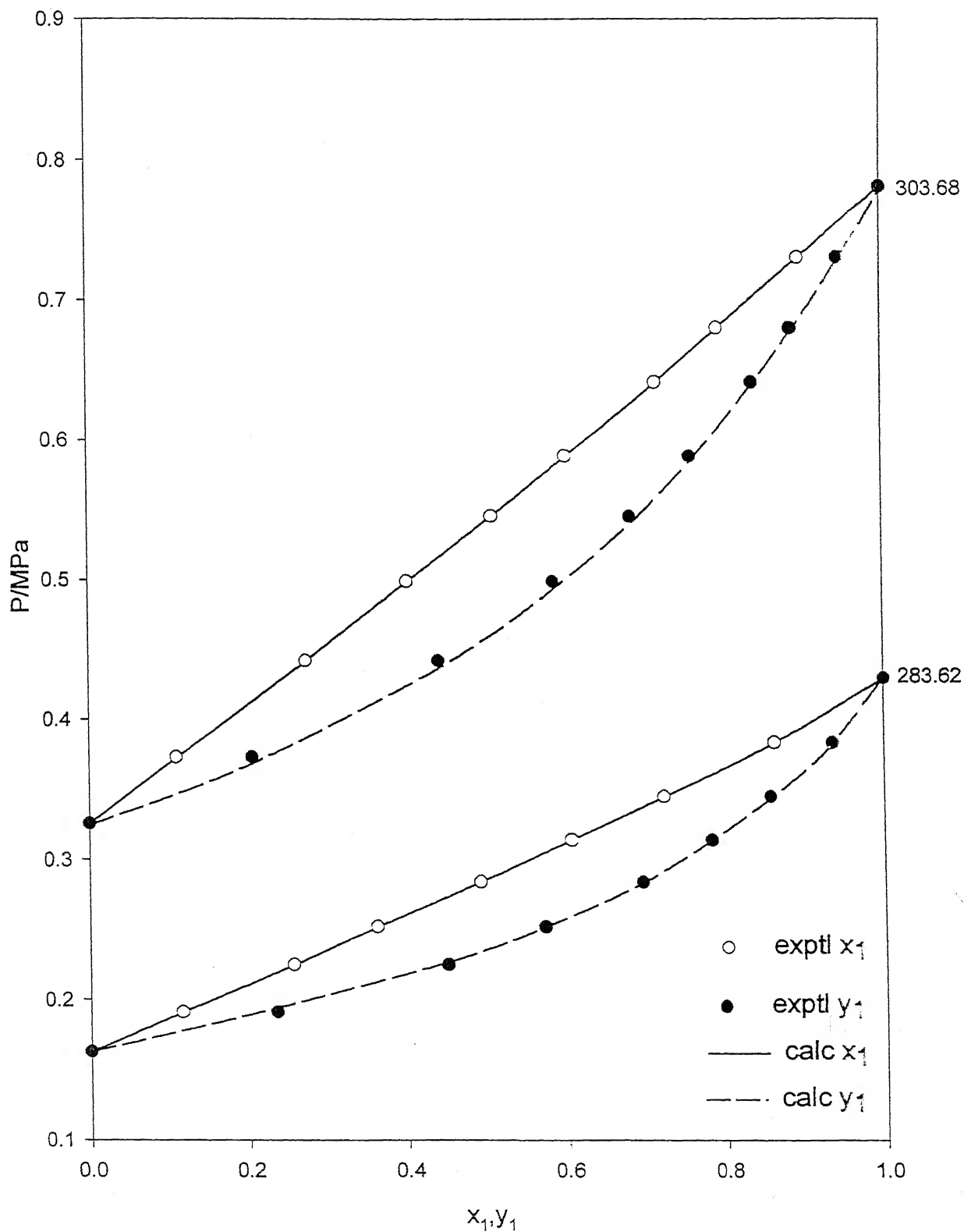


Fig. 4.22 Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-236fa(2) mixtures at different temperatures (K).

Table 4.33: Vapor-liquid equilibrium pressures and phase compositions for R-600a(1)/R-236fa(2) mixtures at 303.68 K with different g^E models.

x_1	y_1		P(MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		NRTL	UNIQUAC
			UNIQUAC-R			UNIQUAC-R
0.000	0.000	0.000	0.000	0.326	0.325	0.325
0.061	0.201	0.194	0.199	0.390	0.389	0.389
0.120	0.302	0.304	0.316	0.437	0.434	0.437
0.219	0.408	0.415	0.437	0.483	0.483	0.491
0.265	0.443	0.449	0.472	0.498	0.498	0.507
0.330	0.482	0.488	0.508	0.514	0.514	0.522
0.388	0.510	0.515	0.530	0.523	0.524	0.530
0.490	0.553	0.556	0.555	0.533	0.534	0.536
0.551	0.577	0.578	0.566	0.535	0.536	0.537
0.663	0.624	0.620	0.595	0.535	0.535	0.535
0.715	0.651	0.643	0.617	0.531	0.532	0.531
0.810	0.707	0.700	0.684	0.517	0.517	0.511
0.898	0.791	0.786	0.791	0.487	0.487	0.476
0.958	0.892	0.887	0.900	0.449	0.449	0.440
1.000	1.000	1.000	1.000	0.411	0.410	0.410
	%AAD	0.926	3.012	%AAD	0.237	0.810
						0.809

$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$

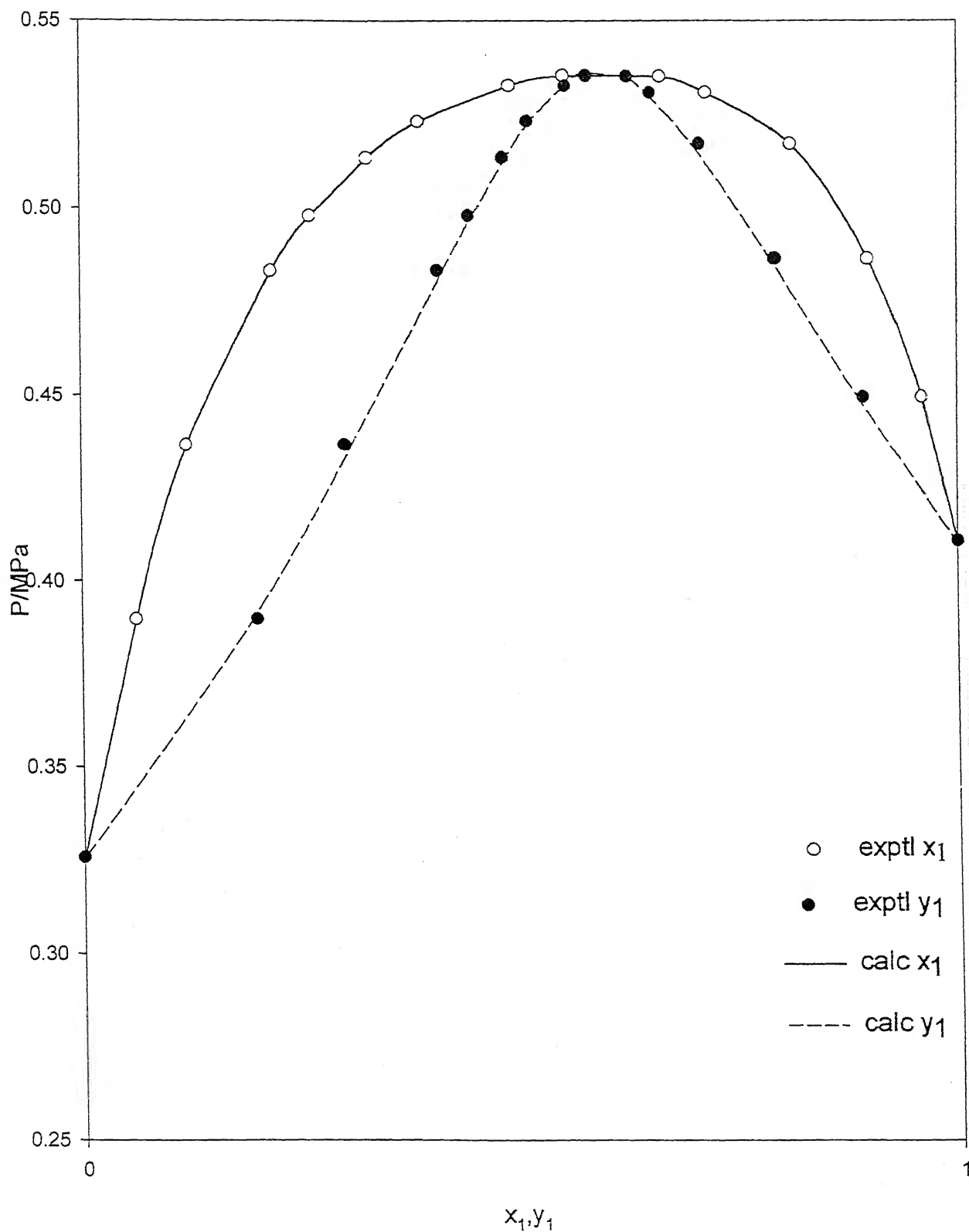


Fig. 4.23 Vapor-liquid equilibrium pressures and phase compositions for R-600a(1)/R-236fa(2) mixtures at 303.68 K.

Table 4.34: Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-23(2) mixtures with different g^E models (contd.).

x ₁	y ₁		P(MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		UNIQUAC-R	NRTL
273.15 K						
0.000	0.000	0.000	0.000	0.495	0.489	0.488
0.102	0.346	0.363	0.346	0.715	0.708	0.702
0.197	0.514	0.529	0.514	0.905	0.905	0.905
0.351	0.677	0.680	0.677	1.205	1.217	1.240
0.510	0.780	0.778	0.780	1.515	1.515	1.556
0.654	0.853	0.846	0.866	1.800	1.761	1.799
0.787	0.906	0.903	0.912	2.065	1.978	2.003
0.867	0.940	0.938	0.941	2.205	2.111	2.126
0.934	0.969	0.968	0.968	2.355	2.229	2.237
1.000	1.000	1.000	1.000	2.501	2.483	2.488
	%AAD	1.129	1.810	%AAD	2.247	2.390
293.15 K						
0.000	0.000	0.000	0.000	0.906	0.897	0.876
0.064	0.207	0.203	0.207	1.110	1.108	1.139
0.196	0.455	0.452	0.455	1.505	1.507	1.503
0.362	0.632	0.630	0.628	2.000	2.000	1.981
0.531	0.744	0.748	0.755	2.495	2.497	2.495
0.693	0.833	0.837	0.845	2.995	2.995	3.006
0.841	0.910	0.947	0.949	3.500	3.745	3.749
0.928	0.955	0.957	0.958	3.850	3.814	3.817
1.000	1.000	1.000	1.000	4.123	4.142	4.115
	%AAD	2.375	3.375	%AAD	1.192	1.719
						0.895
						1.139
						1.503
						1.981
						2.495
						3.006
						3.749
						3.817
						4.115
						1.720

Table 4.34: Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-23(2) mixtures with different g^E models.

x_1	y_1		$P(\text{MPa})$			
	exptl	calc		calc		
		NRTL	UNIQUAC	UNIQUAC-R	NRTL	UNIQUAC
						UNIQUAC-R

303.15 K

0.000	0.000	0.000	0.000	0.000	0.000	1.188	1.176	1.154	1.164
0.090	0.246	0.236	0.250	0.246	0.246	1.525	1.500	1.575	1.575
0.228	0.467	0.464	0.449	0.467	0.467	2.020	1.990	2.015	2.015
0.367	0.604	0.612	0.598	0.604	0.604	2.510	2.503	2.500	2.500
0.496	0.700	0.710	0.702	0.700	0.700	2.990	2.997	2.990	2.989
0.639	0.781	0.794	0.792	0.781	0.781	3.515	3.566	3.564	3.564
0.755	0.845	0.852	0.852	0.851	0.851	4.000	4.053	4.055	4.051
0.861	0.904	0.911	0.905	0.905	0.905	4.500	4.578	4.568	4.552
0.922	0.936	0.919	0.917	0.917	0.917	4.805	4.788	4.782	4.690
	%AAD	2.046	1.563	1.425	1.425	%AAD	0.847	1.021	1.214

323.15 K

0.000	0.000	0.000	0.000	0.000	1.950	1.943	1.965	1.965
0.098	0.222	0.212	0.215	0.215	2.430	2.419	2.419	2.443
0.218	0.396	0.384	0.382	0.382	3.020	3.008	3.008	3.021
0.327	0.505	0.495	0.491	0.491	3.560	3.560	3.560	3.562
0.412	0.577	0.561	0.559	0.559	3.995	4.001	4.001	3.995
0.524	0.644	0.630	0.630	0.627	4.575	4.597	4.597	4.587
0.604	0.682	0.665	0.667	0.667	4.990	5.017	5.017	5.014
0.641	0.693	0.677	0.675	0.676	5.170	5.187	5.187	5.194
0.660	0.691	0.676	0.680	0.680	5.255	5.244	5.244	5.256
	%AAD	2.649	2.629	2.693	%AAD	0.323	0.323	0.235

$$\%AAI = \text{average absolute deviation} - \text{defined as } (\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100) / N$$

R-22(1)/R-23(2)

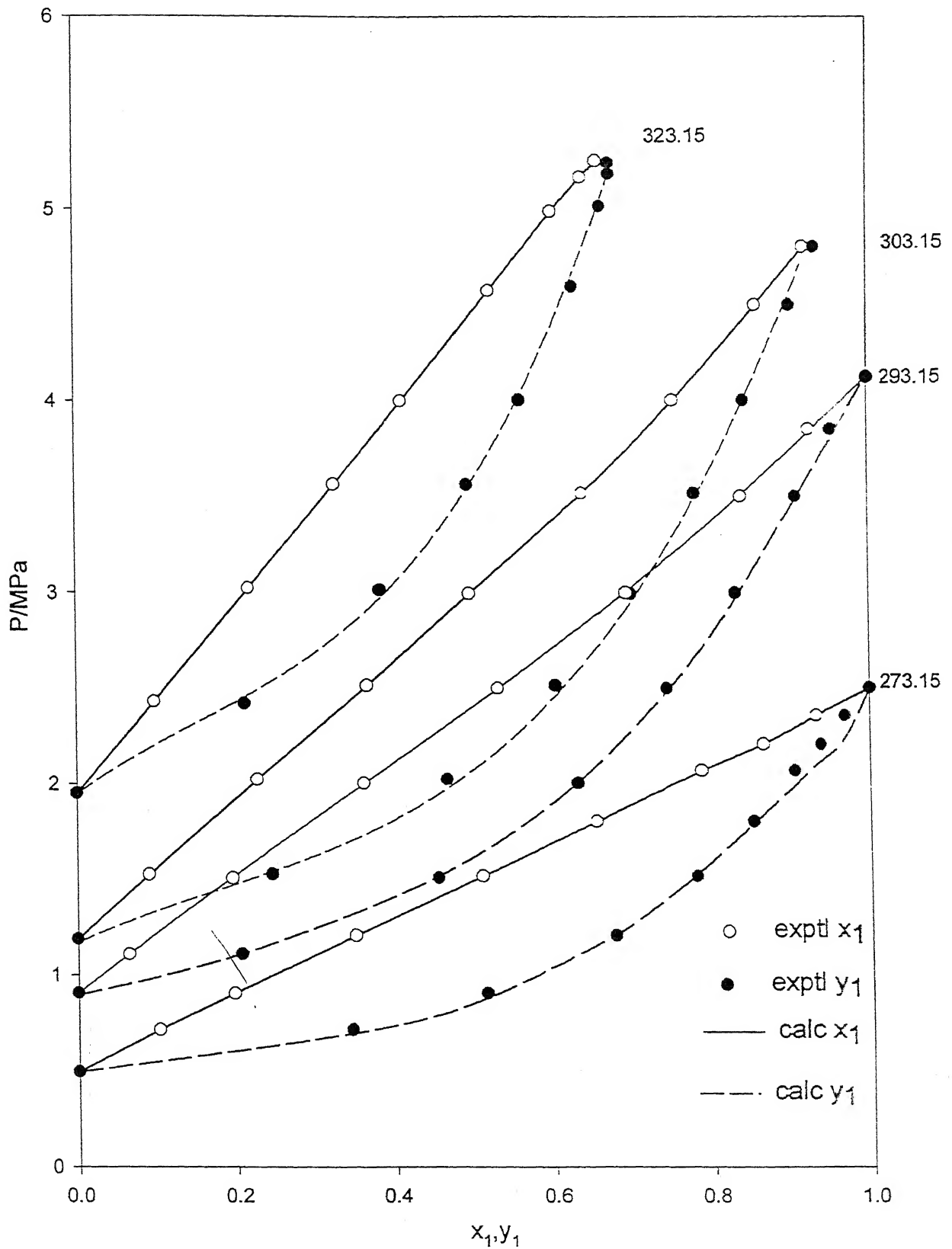


Fig. 4.24 Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-23(2) mixtures at different temperatures (K).

Table 4.35: Vapor-liquid equilibrium pressures and phase compositions for R-152a(1)/R-150a(2) mixtures with different g^E models (contd.).

x_1	y_1		P(MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		NRTL	UNIQUAC
			UNIQUAC-R			UNIQUAC-R
303.2 K						
0.000	0.000	0.000	0.000	0.037	0.037	0.037
0.106	0.693	0.745	0.740	0.134	0.136	0.134
0.194	0.803	0.844	0.842	0.205	0.208	0.207
0.278	0.860	0.888	0.888	0.281	0.271	0.271
0.372	0.891	0.918	0.917	0.336	0.336	0.336
0.528	0.927	0.946	0.945	0.431	0.431	0.431
0.608	0.940	0.957	0.956	0.470	0.477	0.477
0.705	0.953	0.968	0.967	0.530	0.533	0.532
0.799	0.966	0.978	0.977	0.595	0.588	0.587
0.881	0.977	0.987	0.986	0.639	0.639	0.638
0.950	0.985	0.994	0.994	0.685	0.686	0.685
1.000	1.000	1.000	1.000	0.721	0.722	0.721
	%AAD	2.776	2.614	%AAD	1.054	0.788
						1.990

%AAD) average absolute deviation defined as $(\sum abs((exp - calc)/exp) * 100) / N$

Table 4.35: Vapor-liquid equilibrium pressures and phase compositions for R-152a(1)/R-150a(2) mixtures with different g^E models.

x ₁	y ₁				P(MPa)			
	exptl	calc			exptl	calc		
		NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
323.2 K								
0.000	0.000	0.000	0.000	0.000	0.080	0.079	0.079	0.080
0.102	0.634	0.652	0.634	0.637	0.158	0.214	0.201	0.202
0.164	0.758	0.757	0.749	0.753	0.277	0.293	0.277	0.281
0.272	0.825	0.845	0.847	0.851	0.440	0.423	0.408	0.417
0.341	0.855	0.877	0.882	0.886	0.515	0.501	0.490	0.503
0.488	0.902	0.921	0.927	0.931	0.670	0.661	0.659	0.681
0.532	0.911	0.930	0.937	0.940	0.708	0.708	0.708	0.732
0.618	0.928	0.946	0.952	0.955	0.791	0.797	0.800	0.825
0.761	0.952	0.967	0.971	0.973	0.942	0.947	0.950	0.971
0.827	0.964	0.976	0.979	0.980	1.016	1.019	1.020	1.036
0.939	0.982	0.991	0.992	0.992	1.147	1.149	1.149	1.152
1.000	1.000	1.000	1.000	1.000	1.229	1.230	1.230	1.229
	%AAD	1.786	1.981	1.854	%AAD	5.115	4.353	4.424

$$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$$

R-152a(1)/R-150a(2)

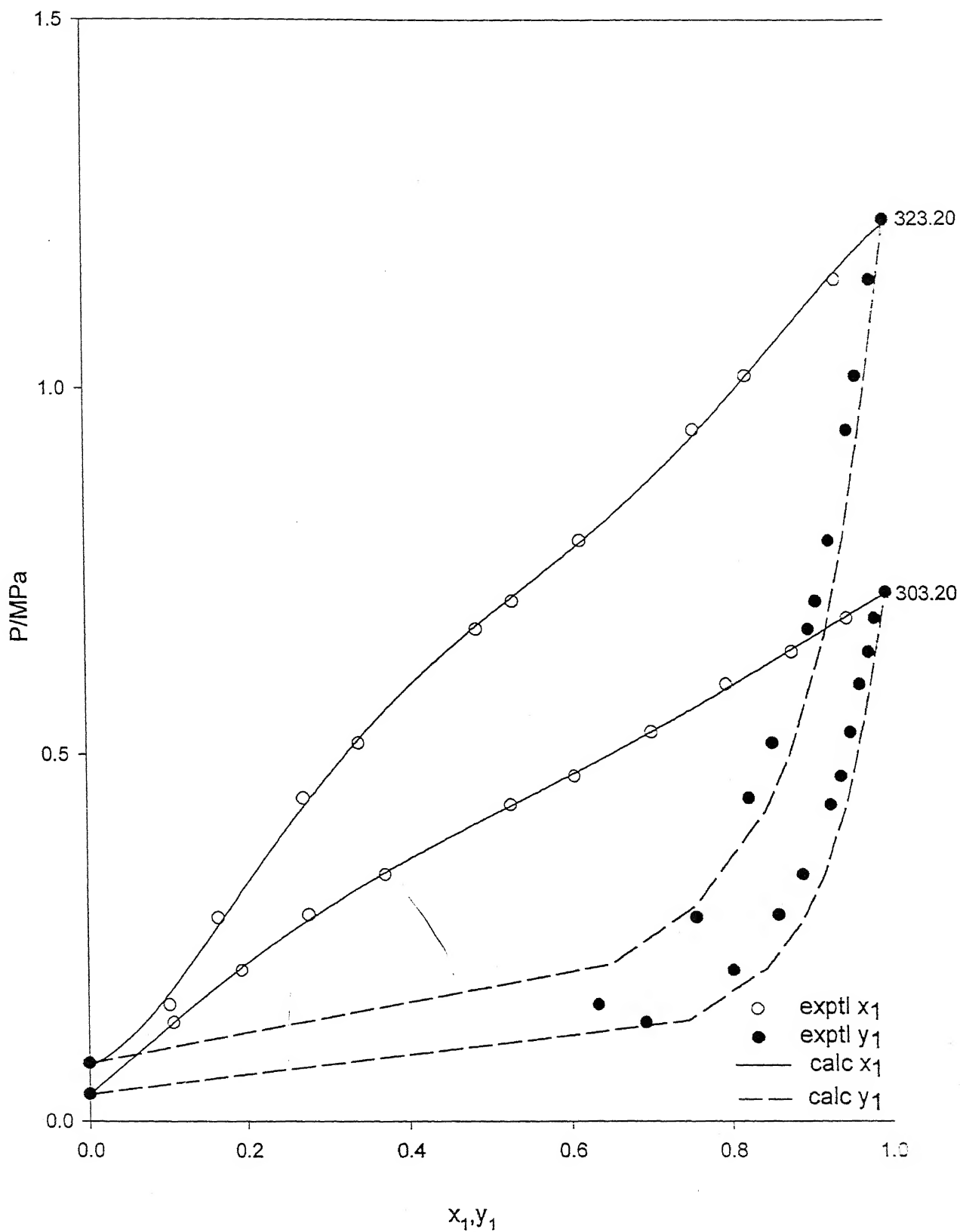


Fig. 4.25 Vapor-liquid equilibrium pressures and phase compositions for R-152a(1)/R-150a(2) mixtures at different temperatures (K).

Table 4.36: Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-142b(2) mixtures with different g^E models (contd.).

x ₁	y ₁		P(MPa)					
	exptl	NRTL	calc		exptl	NRTL	calc	
			UNIQUAC	UNIQUAC-R			UNIQUAC	UNIQUAC-R
268.0 K								
0.000	0.000	0.000	0.000	0.000	0.119	0.119	0.119	0.119
0.182	0.328	0.336	0.335	0.335	0.148	0.149	0.149	0.149
0.274	0.445	0.452	0.450	0.450	0.162	0.162	0.162	0.162
0.374	0.542	0.556	0.555	0.555	0.175	0.176	0.175	0.175
0.470	0.636	0.640	0.640	0.639	0.187	0.187	0.187	0.187
0.572	0.709	0.718	0.720	0.719	0.200	0.199	0.199	0.200
0.701	0.805	0.808	0.808	0.809	0.213	0.213	0.213	0.213
0.837	0.897	0.895	0.895	0.895	0.227	0.226	0.226	0.226
0.950	0.966	0.967	0.967	0.967	0.237	0.237	0.237	0.237
1.000	1.000	1.000	1.000	1.000	0.243	0.241	0.241	0.242
	%AAD	0.946	0.868	0.801	%AAD	0.203	0.198	0.202
283.0 K								
0.000	0.000	0.000	0.000	0.000	0.207	0.206	0.206	0.206
0.088	0.170	0.176	0.175	0.175	0.230	0.230	0.230	0.230
0.173	0.306	0.311	0.309	0.309	0.252	0.252	0.251	0.251
0.268	0.429	0.433	0.433	0.433	0.275	0.275	0.274	0.274
0.364	0.526	0.535	0.538	0.538	0.296	0.297	0.296	0.296
0.467	0.619	0.628	0.633	0.633	0.318	0.318	0.318	0.318
0.560	0.700	0.703	0.708	0.708	0.337	0.336	0.337	0.337
0.692	0.788	0.797	0.799	0.799	0.361	0.360	0.361	0.361
0.832	0.890	0.890	0.890	0.890	0.386	0.384	0.385	0.385
0.951	0.964	0.968	0.968	0.968	0.405	0.403	0.403	0.403
1.000	1.000	1.000	1.000	1.000	0.413	0.411	0.411	0.411
	%AAD	1.035	1.105	1.107	%AAD	0.272	0.191	0.191

%AAD = average absolute deviation - defined as $(\sum \text{abs}(\text{exp} - \text{calc}) / \text{exp}) * 100 / N$

Table 4.36: Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-142b(2) mixtures
with different g^E models.

x ₁	y ₁				P(MPa)			
	exptl	calc			exptl	calc		
		NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
298.0 K								
0.000	0.000	0.000	0.000	0.000	0.337	0.337	0.337	0.337
0.086	0.158	0.164	0.162	0.162	0.370	0.373	0.372	0.372
0.170	0.291	0.295	0.293	0.293	0.404	0.406	0.404	0.404
0.262	0.410	0.415	0.415	0.415	0.439	0.441	0.439	0.439
0.353	0.512	0.513	0.517	0.517	0.472	0.473	0.472	0.472
0.451	0.600	0.605	0.611	0.611	0.505	0.505	0.505	0.505
0.556	0.686	0.692	0.698	0.698	0.539	0.538	0.539	0.539
0.688	0.784	0.788	0.792	0.792	0.578	0.577	0.578	0.578
0.824	0.883	0.882	0.882	0.882	0.617	0.614	0.615	0.615
0.933	0.955	0.955	0.955	0.955	0.644	0.643	0.643	0.643
1.000	1.000	1.000	1.000	1.000	0.662	0.660	0.660	0.660
	%AAD	0.815	0.939	0.942	%AAD	0.309	0.140	0.141

$\%AAD$: average absolute deviation defined as $(\sum abs((exp - calc)/exp) * 100) / N$

Table 4.37: Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-12(2) mixtures with different g^E models (contd.).

x ₁	y ₁			P(MPa)		
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		UNIQUAC-R	NRTL
258.0 K						
0.000	0.000	0.000	0.000	0.182	0.185	0.185
0.122	0.215	0.202	0.203	0.208	0.209	0.208
0.245	0.322	0.314	0.323	0.220	0.220	0.220
0.321	0.375	0.366	0.375	0.223	0.223	0.223
0.489	0.464	0.464	0.458	0.224	0.224	0.224
0.548	0.501	0.496	0.484	0.223	0.223	0.223
0.652	0.559	0.558	0.539	0.219	0.219	0.219
0.762	0.642	0.638	0.623	0.210	0.210	0.209
0.868	0.754	0.745	0.746	0.195	0.196	0.193
1.000	1.000	1.000	1.000	0.163	0.163	0.163
	%AAD	1.412	1.833	%AAD	0.337	0.370
278.0 K						
0.000	0.000	0.000	0.000	0.360	0.358	0.358
0.121	0.211	0.197	0.209	0.409	0.401	0.409
0.239	0.320	0.324	0.328	0.435	0.427	0.435
0.315	0.374	0.387	0.383	0.443	0.438	0.444
0.489	0.484	0.501	0.478	0.450	0.448	0.449
0.550	0.520	0.536	0.509	0.448	0.448	0.448
0.657	0.589	0.599	0.571	0.440	0.443	0.440
0.768	0.675	0.673	0.659	0.425	0.431	0.423
0.870	0.785	0.768	0.775	0.399	0.408	0.396
1.000	1.000	1.000	1.000	0.349	0.347	0.347
	%AAD	2.218	1.587	%AAD	1.081	0.237
						0.234

%AAD = average absolute deviation - defined as $(\sum abs((exp - calc) / exp) * 100) / N$

Table 4.37: Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-12(2) mixtures with different g^E models.

x_1	y_1		P (MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		NRTL	UNIQUAC
						UNIQUAC-R
298.0 K						
0.000	0.000	0.000	0.000	0.648	0.635	0.635
0.110	0.187	0.189	0.193	0.726	0.725	0.723
0.219	0.302	0.297	0.312	0.772	0.773	0.772
0.298	0.368	0.359	0.376	0.794	0.794	0.794
0.488	0.493	0.491	0.493	0.813	0.814	0.814
0.551	0.534	0.535	0.529	0.812	0.812	0.813
0.657	0.609	0.612	0.596	0.802	0.802	0.802
0.773	0.704	0.706	0.690	0.777	0.776	0.775
0.884	0.820	0.821	0.817	0.733	0.733	0.729
1.000	1.000	1.000	1.000	0.662	0.660	0.660
	%AAD	0.640	1.405	%AAD	0.277	0.383

$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$

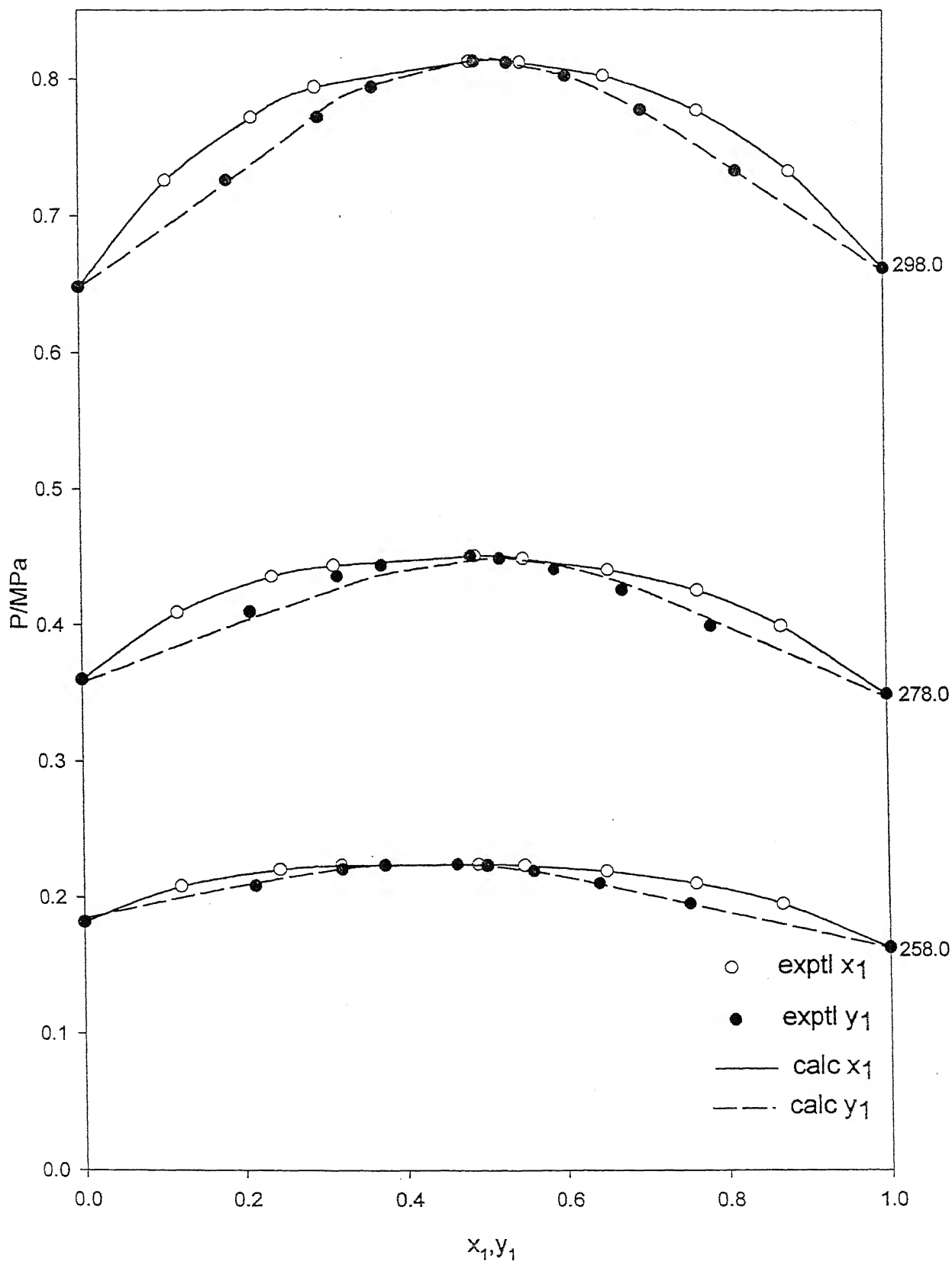


Fig. 4.26 Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-12(2) mixtures at different temperatures (K).

Table 4.38: Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-152a(2) mixtures with different g^E models (contd.).

x ₁	y ₁		P(MPa)				
	exptl	NRTL	calc		exptl	calc	
			UNIQUAC	UNIQUAC-R		UNIQUAC	UNIQUAC-R
255.0 K							
0.000	0.000	0.000	0.000	0.000	0.130	0.129	0.134
0.315	0.330	0.323	0.381	0.381	0.133	0.133	0.125
0.449	0.466	0.467	0.536	0.536	0.134	0.134	0.131
0.550	0.574	0.573	0.626	0.626	0.135	0.135	0.135
0.658	0.674	0.683	0.710	0.710	0.137	0.137	0.139
0.759	0.778	0.783	0.788	0.788	0.139	0.139	0.141
0.884	0.900	0.899	0.892	0.892	0.141	0.141	0.143
1.000	1.000	1.000	1.000	1.000	0.144	0.144	0.144
	%AAD	0.664	5.899	6.738	%AAD	0.055	1.945
							1.821
275.0 K							
0.000	0.000	0.000	0.000	0.000	0.282	0.293	0.293
0.323	0.333	0.329	0.365	0.365	0.288	0.290	0.278
0.448	0.466	0.463	0.508	0.508	0.291	0.292	0.287
0.550	0.575	0.570	0.606	0.606	0.295	0.295	0.295
0.665	0.684	0.687	0.705	0.705	0.298	0.298	0.301
0.759	0.778	0.780	0.784	0.784	0.302	0.301	0.306
0.887	0.898	0.900	0.895	0.895	0.308	0.307	0.310
1.000	1.000	1.000	1.000	1.000	0.313	0.312	0.312
	%AAD	0.460	3.509	3.505	%AAD	0.722	1.470
							1.469

%AAD average absolute deviation defined as $(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100) / N$

Table 4.38: Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-152a(2) mixtures with different g^E models.

x_1	y_1		P (MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		NRTL	UNIQUAC
			UNIQUAC-R			UNIQUAC-R
298.0 K						
0.000	0.000	0.000	0.000	0.594	0.620	0.620
0.320	0.337	0.325	0.334	0.608	0.614	0.608
0.446	0.466	0.460	0.472	0.616	0.618	0.617
0.550	0.569	0.569	0.578	0.623	0.623	0.625
0.663	0.682	0.684	0.688	0.631	0.631	0.635
0.758	0.774	0.777	0.777	0.639	0.638	0.642
0.883	0.894	0.895	0.893	0.651	0.648	0.652
0.978	0.979	0.980	0.979	0.660	0.657	0.658
1.000	1.000	1.000	1.000	0.662	0.660	0.660
	%AAD	0.621	0.589	%AAD	0.813	0.741
			0.586			0.742

$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$

Table 4.39: Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-116(2) mixtures with different g^E models.

x ₁	y ₁		P(MPa)			
	exptl	NRTL	calc		exptl	calc
			UNIQUAC	UNIQUAC-R		
251.0 K						
0.000	0.000	0.000	0.000	0.000	0.980	0.978
0.229	0.092	0.091	0.084	0.084	0.885	0.900
0.322	0.112	0.108	0.097	0.097	0.846	0.868
0.468	0.137	0.128	0.114	0.114	0.779	0.810
0.681	0.178	0.167	0.160	0.160	0.652	0.652
0.762	0.212	0.196	0.196	0.196	0.575	0.555
0.838	0.260	0.246	0.257	0.257	0.476	0.441
0.923	0.396	0.380	0.412	0.412	0.316	0.286
0.976	0.668	0.650	0.690	0.690	0.186	0.175
1.000	1.000	0.998	0.998	0.998	0.121	0.122
	%AAD	3.728	6.383	7.078	%AAD	3.514
						3.877
275.0 K						
0.000	0.000	0.000	0.000	0.000	1.936	1.945
0.700	0.270	0.213	0.243	0.243	1.171	1.190
0.754	0.300	0.250	0.276	0.276	1.068	1.067
0.816	0.359	0.313	0.331	0.331	0.901	0.908
0.894	0.463	0.453	0.454	0.454	0.700	0.677
0.938	0.583	0.595	0.584	0.584	0.557	0.531
0.983	0.818	0.843	0.830	0.830	0.386	0.376
1.000	1.000	0.999	0.999	0.999	0.313	0.312
	%AAD	7.233	3.655	4.843	%AAD	1.733
						2.206

%AAD = average absolute deviation – defined as $(\sum abs((exp - calc) / exp) * 100) / N$

Table 4.40: Vapor-liquid equilibrium pressures and phase compositions for R-134a(1)/R-152a(2) mixtures at 199.80 K with different g^E models.

x_1	y_1		P(MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		NRTL	UNIQUAC
			UNIQUAC-R			UNIQUAC-R
0.000	0.000	0.000	0.000	0.154	0.156	0.156
0.028	0.228	0.243	0.277	0.201	0.203	0.214
0.054	0.381	0.385	0.409	0.245	0.247	0.259
0.119	0.581	0.581	0.579	0.345	0.351	0.355
0.125	0.602	0.592	0.589	0.360	0.360	0.360
0.242	0.753	0.741	0.733	0.532	0.530	0.512
0.362	0.828	0.817	0.816	0.690	0.688	0.671
0.494	0.877	0.870	0.876	0.849	0.852	0.848
0.649	0.917	0.914	0.921	1.035	1.039	1.051
0.778	0.948	0.945	0.950	1.203	1.202	1.215
0.895	0.974	0.973	0.975	1.376	1.362	1.368
1.000	1.000	1.000	1.000	1.527	1.527	1.527
	%AAD	1.186	3.047	3.326	0.609	2.033
				%AAD		1.936

%AAD = average absolute deviation – defined as $(\sum abs((exp - calc) / exp) * 100) / N$

Table 4.41: Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-134a(2) mixtures with different g^E models (contd.).

x_1	y_1		P(MPa)			
	exptl	calc		exptl	calc	
		NRTL	UNIQUAC		NRTL	UNIQUAC
			UNIQUAC-R			UNIQUAC-R
273.16 K						
0.000	0.000	0.000	0.000	0.293	0.292	0.292
0.304	0.421	0.427	0.414	0.364	0.364	0.364
0.413	0.530	0.541	0.532	0.394	0.388	0.386
0.576	0.685	0.687	0.686	0.419	0.421	0.420
0.739	0.812	0.814	0.815	0.451	0.452	0.451
0.824	0.875	0.876	0.877	0.468	0.467	0.467
1.000	1.000	1.000	1.000	0.498	0.497	0.497
	%AAD	0.566	0.427	%AAD	0.393	0.358
298.16 K						
0.000	0.000	0.000	0.000	0.665	0.663	0.663
0.295	0.390	0.392	0.368	0.801	0.795	0.819
0.552	0.644	0.643	0.623	0.897	0.897	0.897
0.746	0.804	0.803	0.799	0.964	0.966	0.959
0.823	0.863	0.863	0.863	0.987	0.991	0.985
1.000	1.000	1.000	1.000	1.045	1.045	1.045
	%AAD	0.140	1.572	%AAD	0.302	0.545
			1.573			0.544

%AAD = average absolute deviation – defined as $(\sum \text{abs}(\text{exp} - \text{calc}) / \text{exp}) * 100 / N$

Table 4.41: Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-134a(2) mixtures with different g^E models.

x_1	y_1				P(MPa)			
	exptl	calc			exptl	calc		
		NRTL	UNIQUAC	UNIQUAC-R		NRTL	UNIQUAC	UNIQUAC-R
323.16 K								
0.000	0.000	0.000	0.000	0.000	1.317	1.318	1.318	1.318
0.300	0.371	0.369	0.366	0.366	1.533	1.526	1.535	1.535
0.403	0.483	0.478	0.474	0.474	1.606	1.597	1.601	1.601
0.566	0.638	0.634	0.632	0.632	1.703	1.703	1.701	1.701
0.743	0.791	0.788	0.788	0.788	1.807	1.811	1.807	1.807
0.825	0.863	0.856	0.857	0.857	1.852	1.857	1.854	1.854
1.000	1.000	1.000	1.000	1.000	1.942	1.950	1.950	1.950
	%AAD	0.499	0.785	0.787	%AAD	0.285	0.168	0.167

$\%AAD = \text{average absolute deviation} - \text{defined as } \left(\sum \text{abs}((\text{exp} - \text{calc}) / \text{exp}) * 100 \right) / N$

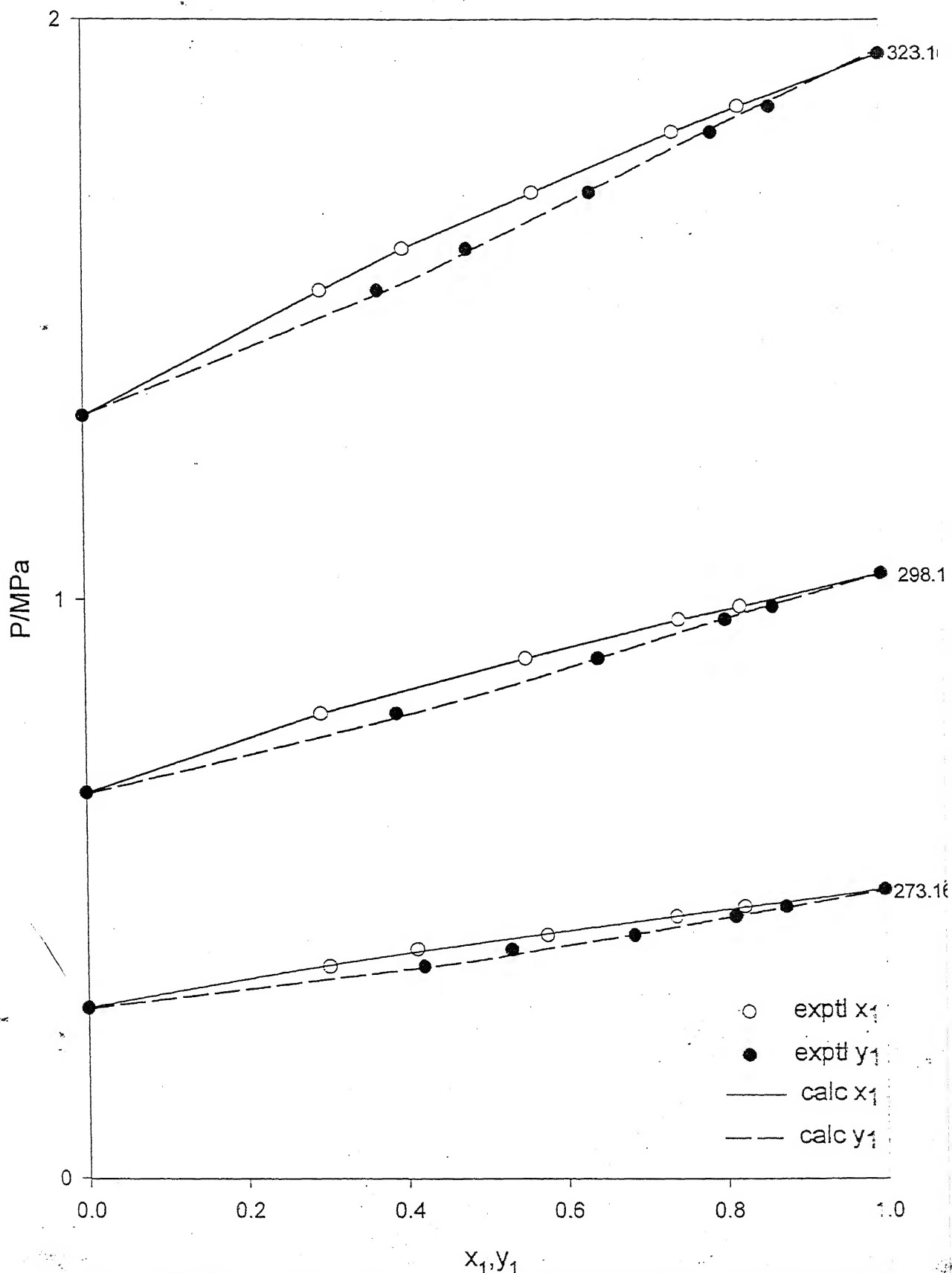


Fig. 4.27 Vapor-liquid equilibrium pressures and phase compositions for R-22(1)/R-134a(2) mixtures at different temperatures (K).

through 4.7 provide comparisons of the fitted WS model using the NRTL equation with the measured total pressure for these systems.

Tables 4.9 through 4.41 give the VLE results for 32 systems for which P-x-y data were available; calculated pressures and vapor mole fractions are compared with the respective experimental values and overall average absolute deviations (%AAD) are presented. Figures 4.8 through 4.27 provide comparisons of the fitted WS model using the NRTL equation with the measured total pressure and vapor composition for some selected systems included in Table 4.9 through 4.41.

The present study reveals that the WS model using any of the three G^E equations allows, in general, accurate representation of phase behavior for a variety of refrigerant mixtures over a range of temperatures and pressures. Moreover, it is interesting to note that the results with the UNIQUAC-R model are comparable to those obtained with the UNIQUAC model, signifying that the combinatorial term has little influence on the accuracy of VLE predictions over the pressure range of interest.

4.4 Conclusions

The results showed that the Wong-Sandler mixing rules with the NRTL, UNIQUAC or UNIQUAC-R activity coefficient models in all cases could be accurately fitted to binary refrigerant VLE data. However, when using this model it is important that the appropriate initial guesses be made for the mixing rule parameter, k_{12} , and the G^E model parameters, τ_{12} , τ_{21} . Although the parameters in the models are slightly temperature dependent, reasonably good predictions can be achieved at other temperatures even if these parameters are assumed to be temperature independent. This would allow extrapolation to higher and lower temperatures when a very limited amount of experimental data are available for a system. Where VLE data exist for more than one temperature, simultaneously fitting the data at all temperatures should provide the best parameters to use over the entire temperature range. Additional calculations and predictions should be

made to further verify this conclusion. Another alternative would be to simultaneously fit VLE along one isotherm and excess enthalpy data, if such data were available.

In summary, on the basis of the results presented here, the WS model appears to be promising in correlation and extrapolation of the vapor-liquid equilibria of refrigerant mixtures over a range of temperatures and pressures, especially for the newer and unconventional mixtures now under consideration.

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